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PASSWORD:

TERMINAL (ENTER 1, 2, 3, OR ?):2

* * * * * Welcome to STN International * * * * *

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500,000 in Key STN Databases
NEWS 3 APR 02 PATDPAFULL: Application and priority number formats
enhanced
NEWS 4 APR 02 DWPI: New display format ALLSTR available
NEWS 5 APR 02 New Thesaurus Added to Derwent Databases for Smooth
Sailing through U.S. Patent Codes
NEWS 6 APR 02 EMBASE Adds Unique Records from MEDLINE, Expanding
Coverage back to 1948
NEWS 7 APR 07 CA/CAPLUS CLASS Display Streamlined with Removal of
Pre-IPC 8 Data Fields
NEWS 8 APR 07 50,000 World Traditional Medicine (WTM) Patents Now
Available in CAPLUS
NEWS 9 APR 07 MEDLINE Coverage Is Extended Back to 1947
NEWS 10 JUN 16 WPI First View (File WPIFV) will no longer be
available after July 30, 2010
NEWS 11 JUN 18 DWPI: New coverage - French Granted Patents
NEWS 12 JUN 18 CAS and FIZ Karlsruhe announce plans for a new
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NEWS 13 JUN 18 IPC codes have been added to the INSPEC backfile
(1969-2009)
NEWS 14 JUN 21 Removal of Pre-IPC 8 data fields streamline displays
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NEWS 16 JUN 28 Introducing "CAS Chemistry Research Report": 40 Years
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Patenting and Commercialization of Bioethanol
NEWS 17 JUN 29 Enhanced Batch Search Options in DGENE, USGENE,
and PCTGEN
NEWS 18 JUL 19 Enhancement of citation information in INPADOC
databases provides new, more efficient competitor
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NEWS 19 JUL 26 CAS coverage of global patent authorities has
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NEWS EXPRESS FEBRUARY 15 10 CURRENT WINDOWS VERSION IS V8.4.2,
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***** STN Columbus *****

FILE 'HOME' ENTERED AT 14:43:17 ON 19 AUG 2010

=> fil reg

COST IN U.S. DOLLARS

SINCE FILE

TOTAL

ENTRY

SESSION

FULL ESTIMATED COST

3.08

3.08

FILE 'REGISTRY' ENTERED AT 14:51:24 ON 19 AUG 2010

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STRUCTURE FILE UPDATES: 18 AUG 2010 HIGHEST RN 1236611-52-1

DICTIONARY FILE UPDATES: 18 AUG 2010 HIGHEST RN 1236611-52-1

New CAS Information Use Policies, enter HELP USAGETERMS for details.

TSCA INFORMATION NOW CURRENT THROUGH June 26, 2010.

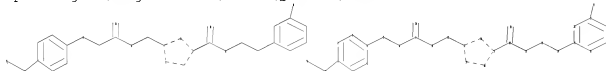
Please note that search-term pricing does apply when conducting SmartSELECT searches.

REGISTRY includes numerically searchable data for experimental and predicted properties as well as tags indicating availability of experimental property data in the original document. For information on property searching in REGISTRY, refer to:

<http://www.cas.org/support/stngen/stdoc/properties.html>

=>

Uploading C:\Program Files\STNEXP\Queries\10598911s.str



```

chain nodes :
7 8 9 10 11 13 14 15 20 21 22 23 25 31
ring nodes :
1 2 3 4 5 6 12 16 17 18 19 24 26 27 28 29 30
chain bonds :
1-13 4-7 7-8 8-9 9-10 9-15 10-11 11-12 13-14 17-20 20-21 20-25 21-22
22-23 23-24 27-31
ring bonds :
1-2 1-6 2-3 3-4 4-5 5-6 12-16 12-19 16-17 17-18 18-19 24-26 24-30
26-27 27-28 28-29 29-30
exact/norm bonds :
1-13 4-7 7-8 9-10 9-15 10-11 12-16 12-19 16-17 17-18 18-19 20-21 20-25
21-22
exact bonds :
8-9 11-12 13-14 17-20 22-23 23-24 27-31
normalized bonds :
1-2 1-6 2-3 3-4 4-5 5-6 24-26 24-30 26-27 27-28 28-29 29-30

```

```

Match level :
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:CLASS 8:CLASS 9:CLASS 10:CLASS
11:CLASS 12:Atom 13:CLASS 14:CLASS 15:CLASS 16:Atom 17:Atom 18:Atom
19:Atom 20:CLASS 21:CLASS 22:CLASS 23:CLASS 24:Atom 25:CLASS 26:Atom
27:Atom 28:Atom 29:Atom 30:Atom 31:CLASS

```

L1 STRUCTURE UPLOADED

=> d

L1 HAS NO ANSWERS

L1 STR

*** STRUCTURE DIAGRAM IS NOT AVAILABLE ***

Structure attributes must be viewed using STN Express query preparation.

=> s l1

SAMPLE SEARCH INITIATED 14:51:44 FILE 'REGISTRY'

SAMPLE SCREEN SEARCH COMPLETED - 21 TO ITERATE

100.0% PROCESSED 21 ITERATIONS

0 ANSWERS

SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **COMPLETE**

BATCH **COMPLETE**

PROJECTED ITERATIONS: 146 TO 694

PROJECTED ANSWERS: 0 TO 0

L2 0 SEA SSS SAM L1

=> s l1 ful

FULL SEARCH INITIATED 14:51:47 FILE 'REGISTRY'

FULL SCREEN SEARCH COMPLETED - 411 TO ITERATE

100.0% PROCESSED 411 ITERATIONS

4 ANSWERS

SEARCH TIME: 00.00.01

L3 4 SEA SSS FUL L1

=> fil caplus

COST IN U.S. DOLLARS

SINCE FILE

TOTAL

FULL ESTIMATED COST

ENTRY
191.54

SESSION
194.62

FILE 'CAPLUS' ENTERED AT 14:51:50 ON 19 AUG 2010
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FILE COVERS 1907 - 19 Aug 2010 VOL 153 ISS 8
FILE LAST UPDATED: 18 Aug 2010 (20100818/ED)
REVISED CLASS FIELDS (/NCL) LAST RELOADED: Jun 2010
USPTO MANUAL OF CLASSIFICATIONS THESAURUS ISSUE DATE: Jun 2010

CAPLUS now includes complete International Patent Classification (IPC) reclassification data for the third quarter of 2010.

CAS Information Use Policies apply and are available at:

<http://www.cas.org/legal/infopolicy.html>

This file contains CAS Registry Numbers for easy and accurate substance identification.

=> s l3

L4 1 L3

=> d ibib abs hitstr tot

=> fil reg		
COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	6.31	200.93
DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)	SINCE FILE ENTRY	TOTAL SESSION
CA SUBSCRIBER PRICE	-0.85	-0.85

FILE 'REGISTRY' ENTERED AT 14:52:05 ON 19 AUG 2010
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 DICTIONARY FILE UPDATES: 18 AUG 2010 HIGHEST RN 1236611-52-1

New CAS Information Use Policies, enter HELP USAGETERMS for details.

TSCA INFORMATION NOW CURRENT THROUGH June 26, 2010.

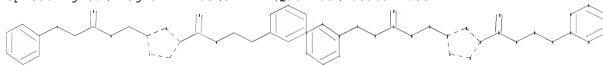
Please note that search-term pricing does apply when conducting SmartSELECT searches.

REGISTRY includes numerically searchable data for experimental and predicted properties as well as tags indicating availability of experimental property data in the original document. For information on property searching in REGISTRY, refer to:

<http://www.cas.org/support/stngen/stndoc/properties.html>

=>

Uploading C:\Program Files\STNEXP\Queries\10598911.str



```

chain nodes :
7  8  9 10 11 13 18 19 20 21 23
ring nodes :
1  2  3  4  5  6 12 14 15 16 17 22 24 25 26 27 28
chain bonds :
4-7  7-8  8-9  9-10  9-13 10-11 11-12 15-18 18-19 18-23 19-20 20-21 21-22

```

ring bonds :
1-2 1-6 2-3 3-4 4-5 5-6 12-14 12-17 14-15 15-16 16-17 22-24 22-28
24-25 25-26 26-27 27-28
exact/norm bonds :
4-7 7-8 9-10 9-13 10-11 12-14 12-17 14-15 15-16 16-17 18-19 18-23 19-20

exact bonds :
8-9 11-12 15-18 20-21 21-22

normalized bonds :
1-2 1-6 2-3 3-4 4-5 5-6 22-24 22-28 24-25 25-26 26-27 27-28

Match level :
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:CLASS 8:CLASS 9:CLASS 10:CLASS
11:CLASS 12:Atom 13:CLASS 14:Atom 15:Atom 16:Atom 17:Atom 18:CLASS
19:CLASS 20:CLASS 21:CLASS 22:Atom 23:CLASS 24:Atom 25:Atom 26:Atom 27:Atom
28:Atom

L5 STRUCTURE UPLOADED

=> d
L5 HAS NO ANSWERS
L5 STR

*** STRUCTURE DIAGRAM IS NOT AVAILABLE ***

Structure attributes must be viewed using STN Express query preparation.

=> s l5
SAMPLE SEARCH INITIATED 15:01:33 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED - 5 TO ITERATE

100.0% PROCESSED 5 ITERATIONS 4 ANSWERS
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **COMPLETE**
BATCH **COMPLETE**
PROJECTED ITERATIONS: 5 TO 234
PROJECTED ANSWERS: 4 TO 200

L6 4 SEA SSS SAM L5

=> s l5 ful
FULL SEARCH INITIATED 15:01:36 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED - 96 TO ITERATE

100.0% PROCESSED 96 ITERATIONS 52 ANSWERS
SEARCH TIME: 00.00.01

L7 52 SEA SSS FUL L5

=> fil caplus
COST IN U.S. DOLLARS SINCE FILE TOTAL

FULL ESTIMATED COST	ENTRY 198.89	SESSION 399.82
DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)	SINCE FILE ENTRY	TOTAL SESSION
CA SUBSCRIBER PRICE	0.00	-0.85

FILE 'CAPLUS' ENTERED AT 15:01:38 ON 19 AUG 2010
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 USPTO MANUAL OF CLASSIFICATIONS THESAURUS ISSUE DATE: Jun 2010

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=> s l7
 L8 1 L7

=> fil reg		
COST IN U.S. DOLLARS	SINCE FILE	TOTAL
	ENTRY	SESSION
FULL ESTIMATED COST	0.50	400.32
DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)	SINCE FILE	TOTAL
	ENTRY	SESSION
CA SUBSCRIBER PRICE	0.00	-0.85

FILE 'REGISTRY' ENTERED AT 15:01:43 ON 19 AUG 2010
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DICTIONARY FILE UPDATES: 18 AUG 2010 HIGHEST RN 1236611-52-1

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TSCA INFORMATION NOW CURRENT THROUGH June 26, 2010.

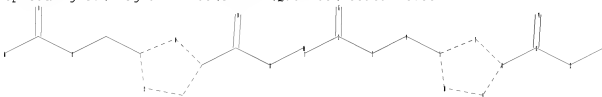
Please note that search-term pricing does apply when
conducting SmartSELECT searches.

REGISTRY includes numerically searchable data for experimental and
predicted properties as well as tags indicating availability of
experimental property data in the original document. For information
on property searching in REGISTRY, refer to:

<http://www.cas.org/support/stngen/stdoc/properties.html>

=>

Uploading C:\Program Files\STNEXP\Queries\10598911b.str



chain nodes :

1 2 3 4 6 11 12 13 14

ring nodes :

5 7 8 9 10

chain bonds :

1-2 2-3 2-6 3-4 4-5 8-11 11-12 11-14 12-13

ring bonds :

5-7 5-10 7-8 8-9 9-10

exact/norm bonds :

1-2 2-3 2-6 3-4 5-7 5-10 7-8 8-9 9-10 11-12 11-14 12-13

exact bonds :

4-5 8-11

Match level :

1:CLASS 2:CLASS 3:CLASS 4:CLASS 5:Atom 6:CLASS 7:Atom 8:Atom 9:Atom
10:Atom 11:CLASS 12:CLASS 13:CLASS 14:CLASS

L9 STRUCTURE UPLOADED

=> d

L9 HAS NO ANSWERS

L9

STR



Structure attributes must be viewed using STN Express query preparation.

=> s l9

SAMPLE SEARCH INITIATED 15:04:30 FILE 'REGISTRY'

SAMPLE SCREEN SEARCH COMPLETED - 507 TO ITERATE

100.0% PROCESSED 507 ITERATIONS

50 ANSWERS

INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED)

SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **COMPLETE**

BATCH **COMPLETE**

PROJECTED ITERATIONS: 8790 TO 11490

PROJECTED ANSWERS: 592 TO 1448

L10

50 SEA SSS SAM L9

=> s l9 ful

FULL SEARCH INITIATED 15:04:33 FILE 'REGISTRY'

FULL SCREEN SEARCH COMPLETED - 9877 TO ITERATE

100.0% PROCESSED 9877 ITERATIONS

1053 ANSWERS

SEARCH TIME: 00.00.01

L11

1053 SEA SSS FUL L9

=> fil caplus

COST IN U.S. DOLLARS

SINCE FILE

TOTAL

ENTRY

SESSION

FULL ESTIMATED COST

193.50

593.82

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)

SINCE FILE

TOTAL

ENTRY

SESSION

CA SUBSCRIBER PRICE

0.00

-0.85

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FILE COVERS 1907 - 19 Aug 2010 VOL 153 ISS 8
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REVISED CLASS FIELDS (/NCL) LAST RELOADED: Jun 2010
USPTO MANUAL OF CLASSIFICATIONS THESAURUS ISSUE DATE: Jun 2010

Caplus now includes complete International Patent Classification (IPC) reclassification data for the third quarter of 2010.

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=> s l11
L12 217 L11

=> fil reg		
COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	0.50	594.32
DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)	SINCE FILE ENTRY	TOTAL SESSION
CA SUBSCRIBER PRICE	0.00	-0.85

FILE 'REGISTRY' ENTERED AT 15:04:41 ON 19 AUG 2010
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STRUCTURE FILE UPDATES: 18 AUG 2010 HIGHEST RN 1236611-52-1
DICTIONARY FILE UPDATES: 18 AUG 2010 HIGHEST RN 1236611-52-1

New CAS Information Use Policies, enter HELP USAGETERMS for details.

TSCA INFORMATION NOW CURRENT THROUGH June 26, 2010.

Please note that search-term pricing does apply when conducting SmartSELECT searches.

REGISTRY includes numerically searchable data for experimental and predicted properties as well as tags indicating availability of experimental property data in the original document. For information on property searching in REGISTRY, refer to:

<http://www.cas.org/support/stngen/stndoc/properties.html>

=> fil reg

COST IN U.S. DOLLARS

SINCE FILE	TOTAL
ENTRY	SESSION
1.47	595.79

FULL ESTIMATED COST

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)

SINCE FILE	TOTAL
ENTRY	SESSION
0.00	-0.85

CA SUBSCRIBER PRICE

FILE 'REGISTRY' ENTERED AT 15:06:40 ON 19 AUG 2010
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STRUCTURE FILE UPDATES: 18 AUG 2010 HIGHEST RN 1236611-52-1
DICTIONARY FILE UPDATES: 18 AUG 2010 HIGHEST RN 1236611-52-1

New CAS Information Use Policies, enter HELP USAGETERMS for details.

TSCA INFORMATION NOW CURRENT THROUGH June 26, 2010.

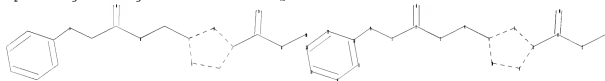
Please note that search-term pricing does apply when conducting SmartSELECT searches.

REGISTRY includes numerically searchable data for experimental and predicted properties as well as tags indicating availability of experimental property data in the original document. For information on property searching in REGISTRY, refer to:

<http://www.cas.org/support/stngen/stndoc/properties.html>

=>

Uploading C:\Program Files\STNEXP\Queries\10598911c.str



```

chain nodes :
1  2  3  4  6  11 12 13 14 15
ring nodes :
5  7  8  9 10 16 17 18 19 20 21
chain bonds :
1-2 1-15 2-3 2-6 3-4 4-5 8-11 11-12 11-14 12-13 15-16
ring bonds :
5-7 5-10 7-8 8-9 9-10 16-17 16-21 17-18 18-19 19-20 20-21
exact/norm bonds :
1-15 2-3 2-6 3-4 5-7 5-10 7-8 8-9 9-10 11-12 11-14 12-13 15-16
exact bonds :
1-2 4-5 8-11
normalized bonds :
16-17 16-21 17-18 18-19 19-20 20-21

```

```

Match level :
1:CLASS 2:CLASS 3:CLASS 4:CLASS 5:Atom 6:CLASS 7:Atom 8:Atom 9:Atom
10:Atom 11:CLASS 12:CLASS 13:CLASS 14:CLASS 15:CLASS 16:Atom 17:Atom
18:Atom 19:Atom 20:Atom 21:Atom

```

L13 STRUCTURE UPLOADED

```

=> d
L13 HAS NO ANSWERS
L13 STR
*** STRUCTURE DIAGRAM IS NOT AVAILABLE ***

```

Structure attributes must be viewed using STN Express query preparation.

```

=> s l13
SAMPLE SEARCH INITIATED 15:06:58 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED - 52 TO ITERATE

100.0% PROCESSED 52 ITERATIONS 15 ANSWERS
SEARCH TIME: 00.00.01

```

```

FULL FILE PROJECTIONS: ONLINE **COMPLETE**
                        BATCH **COMPLETE**
PROJECTED ITERATIONS: 608 TO 1472
PROJECTED ANSWERS: 68 TO 532

```

L14 15 SEA SSS SAM L13

```

=> s l13 ful
FULL SEARCH INITIATED 15:07:01 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED - 1069 TO ITERATE

```

```

100.0% PROCESSED 1069 ITERATIONS 203 ANSWERS
SEARCH TIME: 00.00.01

```

L15 203 SEA SSS FUL L13

=> fil caplus
COST IN U.S. DOLLARS

SINCE FILE	TOTAL
ENTRY	SESSION
191.54	787.33

FULL ESTIMATED COST

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)

SINCE FILE	TOTAL
ENTRY	SESSION
0.00	-0.85

CA SUBSCRIBER PRICE

FILE 'CAPLUS' ENTERED AT 15:07:03 ON 19 AUG 2010
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FILE COVERS 1907 - 19 Aug 2010 VOL 153 ISS 8
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REVISED CLASS FIELDS (/NCL) LAST RELOADED: Jun 2010
USPTO MANUAL OF CLASSIFICATIONS THESAURUS ISSUE DATE: Jun 2010

CAPLUS now includes complete International Patent Classification (IPC) reclassification data for the third quarter of 2010.

CAS Information Use Policies apply and are available at:

<http://www.cas.org/legal/infopolicy.html>

This file contains CAS Registry Numbers for easy and accurate substance identification.

=> s l15
L16 5 L15

=> d ibib abs hitstr tot

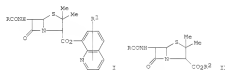
116 NUMBER 2 OF 5 CAPLUS COPYRIGHT 2010 ACS on STM (Continued)

[illegible]

OTHER SOURCE(S): MARPAT 118:191729
GZ

[illegible]

16. ANKHEM 4 OF 5
ACCESSION NUMBER: 1978;170968 CAPLUS
DOCUMENT NUMBER: 88;170915
ORIGINAL SYNTHESE NO.: 88-28010,28010
TITLE: Application of 8-hydroxyguanosine in the synthesis of semi-synthetic 8-azido nucleoside antibiotics and their salts
AUTHOR(S): Starckova, Veronika Mikulskova, Latvya; E. Farkas, Elisabeth; Sopman, Jozsef
CORPORATE SOURCE: Dep. Org. Chem., Lajos Kossuth Univ., Debrecen, Hungary
NOTE: 8-azido nucleoside antibiotics (1977), 94(2); 159-76
COUNTRY ACQNR: USSR; 0001-5407
DOCUMENT TYPE: English
LANGUAGE: English



XZ Esters I = benzyl, PhOCH₂, 3-methyl-3-phenyl-1-isoxanzolyl;
 2-thienylmethyl, 2-(6-Methoxyhexyloxy); X1 = H, 4-Me, 5-Et, 3-ND, 6-Me)
 were prepared in 71-73% yields by reaction of the penicillins derivat
 with the resp. 8-quinolizol. I was effective in vitro against Mycobacter
 sensu stricto, M. fortuitum, M. goodii and streptomycin resistant tuberculo
 sis strains. I was used for the synthesis of II (R = 3-thienylmethyl),
 CICKet,
 ZT R = Et; R = 2-thienylmethyl, PhOCH₂, ND = CH(CH₃)₂.
 66302-15-2P
 XI K2 SFO (Synthetic preparation); PREP (Preparation
 [preparation of
 XU 66302-15-2P CAPUSU
 2-Thiazolidineacetamide,
 1,4-dimethyl-5-[2-oxoox-2-(tricyclo[3.1.1]hept-
 2-ylamino)ethyl]-6-[[2-oxo-2-(tricyclo[3.1.1]hept-
 2-ylamino)ethyl]amino]carbamate]; 1-(2-phenoxyethyl)amino-
 1,3,4,4d'-[C(=O)NHMe]Me

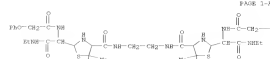
Absolute stereochemistry.

L16 ANMESEK 3 OF 5 CAPLUS COPYRIGHT 2010 ACS ON STM (Continued)
Thiazolidinacetamide; ICI. It inhibited HIV protease with EC50 ≤ 100
nM.

JT 146554-31-1P
[Biological]
ICI: RAC [Biological activity or function, except adverse]; ECU
study, unclassified); SHW (Synthetic preparation); THO (Therapeutic use);
RTOI (Biological study); PREP (Preparation); USES (Uses)
[Preparation of, as vehicle]

FBI 146554-31-3 CAPLUS

CN 2-Thiazolidinacetamide, 4,4'-[1,2-ethanediyl]bis[(aminocarbonyl)bis[N-(
ethyl-2-thiazolyl)-N-methyl-L-prolinecarbamoyl]]bis[2-
((E)-2-oxo-1,4-dihydroxybutyl)]-N,N'-dimethyl-N,N'-dicarboxylic acid diester.
[E]-2-oxo-1,4-dihydroxybutyl ester; CICA; INDEX NAME



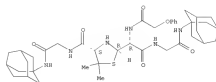
PAGE 7-8

PAGE 1-2

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--CFH

OS.CITING REF COURT: 1  THERE ARE 1 CAPUS RECORDS THAT CITE THIS
RECORD
                        [1 CITINGS]
REFERENCE COURT: 1  THERE ARE 1 CITED REFERENCES AVAILABLE FOR THIS
RECORD. ALL CITATIONS AVAILABLE IN THE RE
FORMAT
```

116 ANSWER 4 OF 5 CAPLOS COPYRIGHT 2010 ACS on STN (Continued)





AB The penicillin esters and amides I (R = Ph, R1 = H, R2 = OMe, OCH2Ph, NMe2, cyclohexylamino, NEPh, NHC6H4Me-3, NHC6H4Me-7, NHC6H4Me-8, R = Ph, R1 = Me, R2 = NMe2, NEPh, NHC6H4Me-3, R = 2,4-Me2C6H3, R1 = Me, R2 = NHC6H4Me-3, R = NMe2, NEPh, NHC6H4Me-3, R = 2,4-Me2C6H3, R1 = Me, R2 = NHC6H4Me-3) were prepared from the triethylamine, Na, or K salts by mixed anhydride method.

II (R = Ph, R1 = H, R2 = OH, OMe, OCH2Ph, NHC6H4Me-3, R = Ph, R1 = Me, R2 = OH, NHC6H4Me-3, R = 2,4-Me2C6H3, 2,4-Me2C6H3, R2 = H, R2 = OH, R = 2,4-Me2C6H3, R1 = Me, R2 = OH, R = 2,4-Me2C6H3, R1 = Me, R2 = NHC6H4Me-3) were obtained by treating the triethylamine salts with Na2CO3.HCl or Na2CO3.HCl.

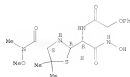
IT 61100-40-12
R1: PH (Synthetic preparation); PREP (Preparation of)

PREP (Preparation of)

PREP (Preparation of)

CH 2-Thiazolidineacetamide, N-hydroxy-4-[[methoxymethylamino]carbonyl]-5,5-dimethyl-4-[[methoxymethylamino]amino]-, [2S-[2a(R'),4P]]-[5C1] (CA INDEX NAME)

Absolute stereochemistry.



=> fil reg		
COST IN U.S. DOLLARS	SINCE FILE	TOTAL
	ENTRY	SESSION
FULL ESTIMATED COST	31.05	818.38
DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)	SINCE FILE	TOTAL
	ENTRY	SESSION
CA SUBSCRIBER PRICE	-4.25	-5.10

FILE 'REGISTRY' ENTERED AT 15:09:12 ON 19 AUG 2010
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STRUCTURE FILE UPDATES: 18 AUG 2010 HIGHEST RN 1236611-52-1
 DICTIONARY FILE UPDATES: 18 AUG 2010 HIGHEST RN 1236611-52-1

New CAS Information Use Policies, enter HELP USAGETERMS for details.

TSCA INFORMATION NOW CURRENT THROUGH June 26, 2010.

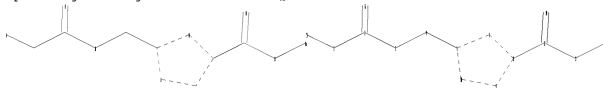
Please note that search-term pricing does apply when
 conducting SmartSELECT searches.

REGISTRY includes numerically searchable data for experimental and
 predicted properties as well as tags indicating availability of
 experimental property data in the original document. For information
 on property searching in REGISTRY, refer to:

<http://www.cas.org/support/stngen/stndoc/properties.html>

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Uploading C:\Program Files\STNEXP\Queries\1059891ld.str



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 1 2 3 4 6 11 12 13 14 15
 ring nodes :
 5 7 8 9 10
 chain bonds :
 1-2 1-15 2-3 2-6 3-4 4-5 8-11 11-12 11-14 12-13
 ring bonds :
 5-7 5-10 7-8 8-9 9-10
 exact/norm bonds :

1-15 2-3 2-6 3-4 5-7 5-10 7-8 8-9 9-10 11-12 11-14 12-13
exact bonds :
1-2 4-5 8-11

Match level :

1:CLASS 2:CLASS 3:CLASS 4:CLASS 5:Atom 6:CLASS 7:Atom 8:Atom 9:Atom
10:Atom 11:CLASS 12:CLASS 13:CLASS 14:CLASS 15:CLASS

L17 STRUCTURE UPLOADED

=> d

L17 HAS NO ANSWERS

L17 STR



Structure attributes must be viewed using STN Express query preparation.

=> s l17

SAMPLE SEARCH INITIATED 15:09:56 FILE 'REGISTRY'

SAMPLE SCREEN SEARCH COMPLETED - 142 TO ITERATE

100.0% PROCESSED 142 ITERATIONS

15 ANSWERS

SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **COMPLETE**

BATCH **COMPLETE**

PROJECTED ITERATIONS: 2126 TO 3554

PROJECTED ANSWERS: 68 TO 532

L18 15 SEA SSS SAM L17

=> s l17 ful

FULL SEARCH INITIATED 15:10:00 FILE 'REGISTRY'

FULL SCREEN SEARCH COMPLETED - 3055 TO ITERATE

100.0% PROCESSED 3055 ITERATIONS

214 ANSWERS

SEARCH TIME: 00.00.01

L19 214 SEA SSS FUL L17

=> fil caplus

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	ENTRY	SESSION
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	ENTRY	SESSION
CA SUBSCRIBER PRICE	0.00	-5.10

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FILE COVERS 1907 - 19 Aug 2010 VOL 153 ISS 8
FILE LAST UPDATED: 18 Aug 2010 (20100818/ED)
REVISED CLASS FIELDS (/NCL) LAST RELOADED: Jun 2010
USPTO MANUAL OF CLASSIFICATIONS THESAURUS ISSUE DATE: Jun 2010

CAPLUS now includes complete International Patent Classification (IPC) reclassification data for the third quarter of 2010.

CAS Information Use Policies apply and are available at:

<http://www.cas.org/legal/infopolicy.html>

This file contains CAS Registry Numbers for easy and accurate substance identification.

=> s l19

L20 5 L19

=> fil reg

COST IN U.S. DOLLARS	SINCE FILE	TOTAL
	ENTRY	SESSION
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CA SUBSCRIBER PRICE	0.00	-5.10

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STRUCTURE FILE UPDATES: 18 AUG 2010 HIGHEST RN 1236611-52-1
DICTIONARY FILE UPDATES: 18 AUG 2010 HIGHEST RN 1236611-52-1

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TSCA INFORMATION NOW CURRENT THROUGH June 26, 2010.

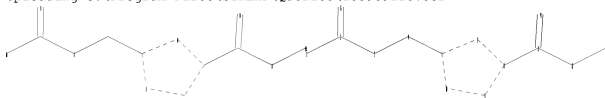
Please note that search-term pricing does apply when conducting SmartSELECT searches.

REGISTRY includes numerically searchable data for experimental and predicted properties as well as tags indicating availability of experimental property data in the original document. For information on property searching in REGISTRY, refer to:

<http://www.cas.org/support/stngen/stndoc/properties.html>

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ring nodes :

5 7 8 9 10

chain bonds :

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ring bonds :

5-7 5-10 7-8 8-9 9-10

exact/norm bonds :

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exact bonds :

4-5 8-11

Match level :

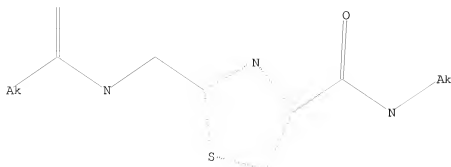
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L21 STRUCTURE UPLOADED

=> d

L21 HAS NO ANSWERS

L21 STR



Structure attributes must be viewed using STN Express query preparation.

=> s l21

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SAMPLE SCREEN SEARCH COMPLETED - 507 TO ITERATE

100.0% PROCESSED 507 ITERATIONS

50 ANSWERS

INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED)

SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **COMPLETE**

BATCH **COMPLETE**

PROJECTED ITERATIONS: 8790 TO 11490

PROJECTED ANSWERS: 592 TO 1448

L22 50 SEA SSS SAM L21

=> s l21 ful

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FULL SCREEN SEARCH COMPLETED - 9877 TO ITERATE

100.0% PROCESSED 9877 ITERATIONS

1053 ANSWERS

SEARCH TIME: 00.00.01

L23 1053 SEA SSS FUL L21

=> fil caplus

COST IN U.S. DOLLARS

SINCE FILE

TOTAL

ENTRY

SESSION

FULL ESTIMATED COST

193.01

1203.43

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)

SINCE FILE

TOTAL

ENTRY

SESSION

CA SUBSCRIBER PRICE

0.00

-5.10

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FILE COVERS 1907 - 19 Aug 2010 VOL 153 ISS 8
FILE LAST UPDATED: 18 Aug 2010 (20100818/ED)
REVISED CLASS FIELDS (/NCL) LAST RELOADED: Jun 2010
USPTO MANUAL OF CLASSIFICATIONS THESAURUS ISSUE DATE: Jun 2010

CAPLUS now includes complete International Patent Classification (IPC) reclassification data for the third quarter of 2010.

CAS Information Use Policies apply and are available at:

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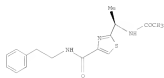
This file contains CAS Registry Numbers for easy and accurate substance identification.

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      23369 THIAZOLE
            (THIAZOLE OR THIAZOLES)
L25          63 L24 AND THIAZOLE

=> s l25 and carboxamide
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L26          4 L25 AND CARBOXAMIDE

=> d ibib abs hitstr tot
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[illegible]

166 AMEREN 2 OF 4 CARLUS 2006131886 2010 ACS on STM
 APPLICATION NUMBER: 2006131886 CARLUS
 DOCUMENT NUMBER: 148-214960
 TITLE: Preparation of anoprogenic compounds with spleen
 tyrosine kinase (Syk)-inhibitory activity
 INVENTOR(S): Kikuchi, Yoshitosh; Waji, Satoru; Matsuda, Kazunori;
 Mizoguchi, Ito, Aoki, Tama; Takata, Hideo; Nakai,
 Yuichi; Ito, Goro; Shinoda, Kiyotaka; Fujiwara,
 Akihiko; Furukawa, Hiroshi; Tanaka, Masaru
 PATENT ASSIGNEE(S): Japan
 SOURCE: PCT Int. Appl., 467pp.
 COUNTRY: PAKIST
 DOCUMENT TYPE: Patent
 LANGUAGE: Japanese
 FAMILY: KCT, INM, COMPTA

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ASSIGNMENT HISTORY FOR US PATENT AVAILABLE IN LEXUS DISPLAY FORMAT

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REFERENCE COURT: 17      THERE ARE 17 CITED REFERENCES AVAILABLE FOR
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RECORD. ALL CITATIONS AVAILABLE IN THE RE
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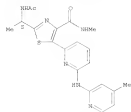
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126 ANSWER 2 OF 4 CAPLOS COPYRIGHT 2010 ACS on STN (Continued)
OTHER SOURCE(S): MARPAT 145:314980
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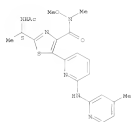
L26 ANMER 2 OF 4 CAPLUS COPYRIGHT 2010 ACS ON STM (Continued)
(Uses)
[prepn. of aminopyridine compds. as spleen tyrosine kinase (Syk)
inhibitors for treatment and/or prevention of allergic diseases]
ZH 90224-40-8 CAPLUS
CH 4-Thiazolocarboxamide, 2-[(12S)-1-(acetylamino)ethyl]-N-methyl-5-[6-[[4-
methyl-2-pyridyl]amino]-2-pyridyl]- (CA INDEX NAME)

Absolute stereochemistry.



ZH 90224-41-5 CAPLUS
CH 4-Thiazolocarboxamide,
2-[(12S)-1-(acetylamino)ethyl]-N-methyl-5-
[6-[[4-methyl-2-pyridyl]amino]-2-pyridyl]- (CA INDEX NAME)

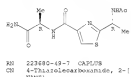
Absolute stereochemistry.



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REFERENCE COUNT: 26 THERE ARE 26 CITED REFERENCES AVAILABLE FOR
THIS
RECORD. ALL CITATIONS AVAILABLE IN THE RE
FORMAT

L16 ANMER 3 OF 4 CAPLUS COPYRIGHT 2010 ACS ON STM
ACCESSION NUMBER: 1999139068 CAPLUS
DOCUMENT NUMBER: 190131089
TITLE: An in silico calculation on peptide-derived oxazoles
AND
thiazoles: improved molecular mechanics
parameters for the AMBER force field
Bader, Christopher D. J.; Mattenden, Gerald
Department of Chemistry, Nottingham University,
Nottingham, NG7 2RD, UK
JOURNAL OF COMPUTER-AIDED MOLECULAR DESIGN (1999),
13(12), 153-166
CODEN JCASDH; ISSN: 0920-654X
PUBLISHER: Kluwer Academic Publishers
DOCUMENT TYPE: Journal
LANGUAGE: English
AB AB in silico calcs. at the RHF/6-31G* and MP2/6-31G**/RHF/6-31G* levels of
theory are performed for 2-methyl-4-oxazolidinone-oxazoles and -
thiazoles, including rotational profiles for the ring-
carboxamide bond, which showed the expected conjugation and
hydrogen bonding effects. On the basis of these data, newly optimized
stretch, bend and torsional parameters for the AMBER force field are
derived, along with CHARMM-fitted partial atomic charges.
IT 221692-45-3 221692-49-7
EI: PEP (Physical, engineering or chemical process); PROC (Process)
lab units calcs. on peptide-derived oxazoles and thiazoles
ZH 221692-45-3 CAPLUS
CH 4-Thiazolocarboxamide, 2-[(12S)-1-(acetylamino)ethyl]-N-[(12S)-2-amino-1-
methyl-2-oxoethyl]- (CA INDEX NAME)

Absolute stereochemistry.



ZH 221692-49-7 CAPLUS
CH 4-Thiazolocarboxamide, 2-[(12S)-1-(acetylamino)ethyl]-N-methyl- (CA INDEX
NAME)

Absolute stereochemistry.

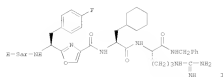


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(5 CITINGS)
REFERENCE COUNT: 44 THERE ARE 44 CITED REFERENCES AVAILABLE FOR
THIS
RECORD. ALL CITATIONS AVAILABLE IN THE RE
FORMAT

L26 ANMER 2 OF 4 CAPLUS COPYRIGHT 2010 ACS ON STM (Continued)

L26 ANMER 3 OF 4 CAPLUS COPYRIGHT 2010 ACS ON STM (Continued)

126 NUMBER 4 OF 4 CAPLUS COPYRIGHT 2010 ACS ON STN (Continued)
 ACCESSION NUMBER: 1999:482687 CAPLUS
 DOCUMENT NUMBER: 123756-41-7
 ORIGINAL REFERENCE NO.: 123756-41-7
 TITLE: Thrombin receptor (PAR-1) antagonists.
 agoniast: Heterocycle-based peptidomimetics of the SPPLR agonist
 AUTHOR(S): Mokhtar, William J.; Hulschier, Becky L.; Mccormay, David F.; Andrade-Ostrows, Patricia; Ruffano, Jack
 A. I.
 ADDN, Michael F.; Chasenberg, Donna; Montbrough, Robert M.; Marganoff, Bruce E.
 CORPATE SOURCE: The W. M. Schaefer Pharmaceutical Research Institute, Spring House, PA, 19477, USA
 SOURCE: Bioorganic & Medicinal Chemistry Letters (1999), 9(13), 2449-2454
 CODEN: BBLE29, ISSN: 0960-894X
 PUBLISHER: Elsevier Science Ltd.
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 GI:

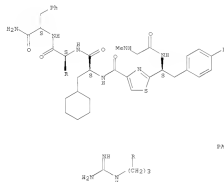


AB The thrombin receptor (PAR-1) is activated by α -thrombin to stimulate various cell types, including platelets, through the tetrapeptide-ligand sequence SPFLRR. A series of oxazole- or thiazole-based oxazolidinones, designed after SPFLR, were synthesized and evaluated in vitro. The compounds inhibited platelet aggregation induced by SPFLRR-NH2 or α -thrombin, and blocked the binding of [18]-Sar-(p-T-FMe)-Sar-Lys-Sar-Lys-Tyr-NH2 (Sar = homocysteine) to a CBP membrane preparation of PAR-1. Oxazole-based peptide 2 bound to PAR-1 with an IC50 of 1.6 μ M, and gave IC50 values of 25 μ M and 6.6 μ M against α -thrombin- and SPFLRR-NH2-induced platelet aggregation, resp.
 IT 212756-41-7P 212756-48-4P 212756-53-3P
 212756-49-5P 212756-50-6P 212756-56-4P
 212756-54-2P 212756-58-6P 212756-59-7P
 212756-60-2P 212756-61-1P 212756-62-2P
 RI, INC (Biological activity or effector, except adverse); RSD (Biochemical study, unclassified); SPH (Synthetic preparation); XCOL (Biological study); PREP (Preparation) (Preparation of oxazole- and thiazole-based peptidomimetics as thrombin receptor antagonists)

126 NUMBER 4 OF 4 CAPLUS COPYRIGHT 2010 ACS ON STN (Continued)
 RI 212756-48-4 CAPLUS
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Absolute stereochemistry.

PAGE 1-A



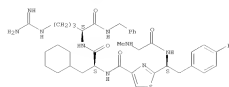
PAGE 2-A

RI 212756-49-5 CAPLUS
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Absolute stereochemistry.

126 NUMBER 4 OF 4 CAPLUS COPYRIGHT 2010 ACS ON STN (Continued)
 RI 212756-41-7 CAPLUS
 CH 1-Arginylamide, N-methylglycyl-2-[(1S)-3-amino-2-(4-fluorophenylethyl)-4-thiazolocarboxyl-3-cyclohexyl-L-alanyl-L-arganyl]- (PCI) (CA INDEX NAME)

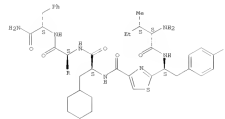
Absolute stereochemistry.



RI 212756-47-3 CAPLUS
 CH 1-Phenylalaninamide, L-isoleucyl-2-[(1S)-3-amino-2-(4-fluorophenylethyl)-4-thiazolocarboxyl-3-cyclohexyl-L-alanyl-L-arganyl]- (PCI) (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A

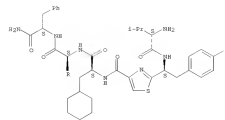


PAGE 2-A



126 NUMBER 4 OF 4 CAPLUS COPYRIGHT 2010 ACS ON STN (Continued)

PAGE 1-A



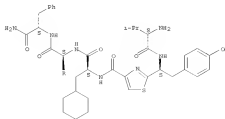
PAGE 2-A

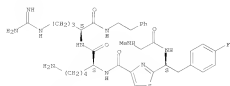


RI 212756-50-8 CAPLUS
 CH 1-Phenylalaninamide, L-valyl-2-[(1S)-3-amino-2-(4-methoxyphenylethyl)-4-thiazolocarboxyl-3-cyclohexyl-L-alanyl-L-arganyl]- (PCI) (CA INDEX NAME)

Absolute stereochemistry.

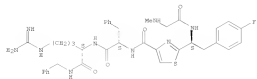
PAGE 1-A





IN 212756-61-1 CAPTUS
 CN L-Arginamide,
 N-methylglycyl-2-((1S)-1-amino-2-(4-fluorophenyl)ethyl)-4-
 thiazolecarboxyl-4-phenylalanyl-8-(phenylmethyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

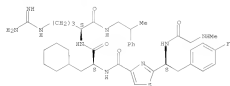


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928 212756-62-2 CAPSUS
CN 1-Argininsanide,
N-methylglycyl-2-[(1S)-1-amino-2-(4-fluorophenyl)ethyl]-4-
thiazolecarboxyl-3-cyclohexyl-L-alanyl-N-(2-phenylpropyl)- (3CI) (CA
INDIC NAME)

```

Absolute stereochemistry.

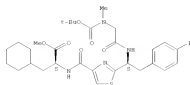


1T 212756-40-6P
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT

L26 ANSWER 4 OF 4 CAPLUS COPYRIGHT 2019 ACS on STN (Contin
(Reactant or reagent)
[prep. of oxazole- and thiazole-based peptidomimetics as
thrombin receptor antagonists]

IN 212756-00-6 CAPLOS
CN Cyclohexanepropanoic acid, α -[[[2-[(1S)-1-[[[1,1-
dimethylethoxy]carbonyl]methylamino]acetyl]amino]-2-(4-fluorophenyl)ethyl]-
4-thiazolyl]carbonyl]amino-, methyl ester, (4S)- (9CI) ICA INDEX
NAME

Absolute stereochemistry.



```
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REFERENCE COUNT: 24  THERE ARE 24 CITED REFERENCES AVAILABLE FOR
THIS
                        RECORD. ALL CITATIONS AVAILABLE IN THE RE
FORMAT
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	ENTRY	SESSION
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	ENTRY	SESSION
CA SUBSCRIBER PRICE	-3.40	-8.50

FILE 'REGISTRY' ENTERED AT 15:13:56 ON 19 AUG 2010
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STRUCTURE FILE UPDATES: 18 AUG 2010 HIGHEST RN 1236611-52-1
 DICTIONARY FILE UPDATES: 18 AUG 2010 HIGHEST RN 1236611-52-1

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TSCA INFORMATION NOW CURRENT THROUGH June 26, 2010.

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 conducting SmartSELECT searches.

REGISTRY includes numerically searchable data for experimental and
 predicted properties as well as tags indicating availability of
 experimental property data in the original document. For information
 on property searching in REGISTRY, refer to:

<http://www.cas.org/support/stngen/stdoc/properties.html>

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CA SUBSCRIBER PRICE	0.00	-8.50

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 provided by InfoChem.

STRUCTURE FILE UPDATES: 18 AUG 2010 HIGHEST RN 1236611-52-1
 DICTIONARY FILE UPDATES: 18 AUG 2010 HIGHEST RN 1236611-52-1

New CAS Information Use Policies, enter HELP USAGETERMS for details.

TSCA INFORMATION NOW CURRENT THROUGH June 26, 2010.

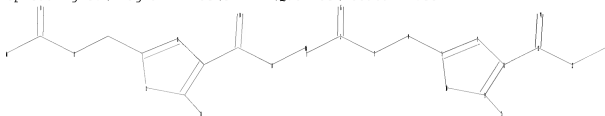
Please note that search-term pricing does apply when conducting SmartSELECT searches.

REGISTRY includes numerically searchable data for experimental and predicted properties as well as tags indicating availability of experimental property data in the original document. For information on property searching in REGISTRY, refer to:

<http://www.cas.org/support/stngen/stdoc/properties.html>

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Uploading C:\Program Files\STNEXP\Queries\10598911f.str



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chain nodes :  
1 2 3 4 6 11 12 13 14 15  
ring nodes :  
5 7 8 9 10  
chain bonds :  
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ring bonds :  
5-7 5-10 7-8 8-9 9-10  
exact/norm bonds :  
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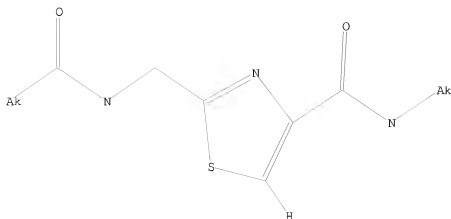
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10:Atom 11:CLASS 12:CLASS 13:CLASS 14:CLASS 15:CLASS

L27 STRUCTURE UPLOADED

=> d

L27 HAS NO ANSWERS

L27 STR



Structure attributes must be viewed using SIN Express query preparation.

=> s l27

SAMPLE SEARCH INITIATED 15:15:37 FILE 'REGISTRY'

SAMPLE SCREEN SEARCH COMPLETED - 507 TO ITERATE

100.0% PROCESSED 507 ITERATIONS

37 ANSWERS

SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **COMPLETE**

BATCH **COMPLETE**

PROJECTED ITERATIONS: 8790 TO 11490

PROJECTED ANSWERS: 376 TO 1104

L28 37 SEA SSS SAM L27

=> s l27 ful

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FULL SCREEN SEARCH COMPLETED - 9877 TO ITERATE

100.0% PROCESSED 9877 ITERATIONS

715 ANSWERS

SEARCH TIME: 00.00.01

L29 715 SEA SSS FUL L27

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COST IN U.S. DOLLARS

SINCE FILE

TOTAL

ENTRY

SESSION

FULL ESTIMATED COST

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DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)

SINCE FILE

TOTAL

ENTRY

SESSION

CA SUBSCRIBER PRICE

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-8.50

FILE 'CAPLUS' ENTERED AT 15:15:42 ON 19 AUG 2010

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FILE COVERS 1907 - 19 Aug 2010 VOL 153 ISS 8
FILE LAST UPDATED: 18 Aug 2010 (20100818/ED)
REVISED CLASS FIELDS (/NCL) LAST RELOADED: Jun 2010
USPTO MANUAL OF CLASSIFICATIONS THESAURUS ISSUE DATE: Jun 2010

CAPLUS now includes complete International Patent Classification (IPC) reclassification data for the third quarter of 2010.

CAS Information Use Policies apply and are available at:

<http://www.cas.org/legal/infopolicy.html>

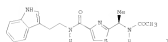
This file contains CAS Registry Numbers for easy and accurate substance identification.

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L30 151 L29

=> s l30 and thiazole
 21400 THIAZOLE
 5238 THIAZOLES
 23369 THIAZOLE
 (THIAZOLE OR THIAZOLES)
L31 53 L30 AND THIAZOLE

=> d ibib abs hitstr tot
THE ESTIMATED COST FOR THIS REQUEST IS 307.93 U.S. DOLLARS
DO YOU WANT TO CONTINUE WITH THIS REQUEST? (Y)/N:y

ACCESSION NUMBER: 2010; 9479 CAPLUS
DOCUMENT NUMBER: 12153757
TITLE: (-)-Bacillamide C: the convergent approach
AUTHOR(S): Wang, Wei; Jeyaraj, Shanmug; Khoury, Karen Andrew
CORPORATE SOURCE: Sumner, David; Alexander, David
Drug Discovery Institute, University of Pittsburgh, Pittsburgh, PA, 15261, USA
SOURCE: 523-333
PUBLISHER: CORDIS; ORCID; ISSN: 1477-0520
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 152357757
GI

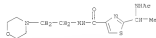


AB The newly discovered natural product bacillamide C (12) and several derivatives were convergently synthesized for the first time and in only three steps. The key transformation constitutes a thiazole Ugi multicomponent reaction. These compounds will serve to elucidate chemical biology and SAR of this potent anti-viral natural product and shows the synthetic pathway to related natural products.

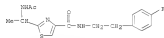
IT 1215381-42-20 CAPLUS
Re: SAR (Biological study, unclassified); STN (Synthetic preparation); RCL (Biological study); PREP (Preparation)
Cellular uptake of preparation of bacillamide C derivative via Ugi multicomponent reaction

RU 1215381-42-2 CAPLUS
CH 4-Thiazolecarboxamide, 2-[1-(acetylamino)ethyl]-8-[2-[[[1-(dimethylamino)-2-[1-(acetylamino)ethyl]-8-[2-(4-morpholinyl)ethyl]-3-naphthyl]amino]ethyl]- (CA INDEX NAME)

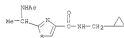
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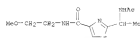
RU 1215381-14-2 CAPLUS
CH 4-Thiazolecarboxamide, 2-[1-(acetylamino)ethyl]-8-[2-(4-fluorophenyl)ethyl]- (CA INDEX NAME)



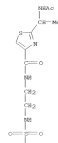
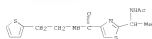
RU 1215381-15-3 CAPLUS
CH 4-Thiazolecarboxamide, 2-[1-(acetylamino)ethyl]-8-[2-(cyclopropylmethyl)- (CA INDEX NAME)



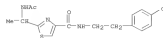
RU 1215381-16-4 CAPLUS
CH 4-Thiazolecarboxamide, 2-[1-(acetylamino)ethyl]-8-[2-(methoxyethyl)- (CA INDEX NAME)



RU 1215381-17-5 CAPLUS
CH 4-Thiazolecarboxamide, 2-[1-(acetylamino)ethyl]-8-[2-(2-thienyl)ethyl]- (CA INDEX NAME)

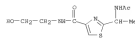


IT 1215381-23-99 1215381-31-99 1215381-34-29
1215381-35-79 1215381-36-49 1215381-37-59
1215381-39-79 1215381-40-09 1215381-44-49
1215381-44-49
Re: STN (Synthetic preparation); PREP (Preparation)
(preparation of bacillamide C derivative via Ugi multicomponent reaction)
RU 1215381-23-9 CAPLUS
CH 4-Thiazolecarboxamide, 2-[1-(acetylamino)ethyl]-8-[2-(4-hydroxyphenyl)ethyl]- (CA INDEX NAME)

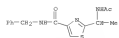


RU 1215381-31-9 CAPLUS

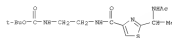
RU 1215381-39-7 CAPLUS
CH 4-Thiazolecarboxamide, 2-[1-(acetylamino)ethyl]-8-[2-(4-hydroxyethyl)- (CA INDEX NAME)



RU 1215381-40-0 CAPLUS
CH 4-Thiazolecarboxamide, 2-[1-(acetylamino)ethyl]-8-[2-(phenylmethyl)- (CA INDEX NAME)

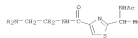


RU 1215381-44-4 CAPLUS
CH Calcium acid, 8-[2-[[[2-[1-(acetylamino)ethyl]-4-thiazolyl]carbonyl]amino]ethyl]-, 1,1-dimethylethyl ester (CA INDEX NAME)



RU 1215381-46-6 CAPLUS
CH 4-Thiazolecarboxamide, 2-[1-(acetylamino)ethyl]-8-[2-(azidoethyl)-, 2,2,2-trifluoroacetate (1:1) (CA INDEX NAME)

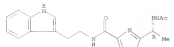
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CH 1215381-45-5
CH C10 H16 N4 O2 S



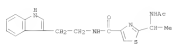
CH 2
CH 76-05-1



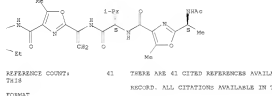
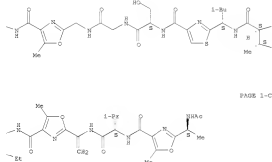
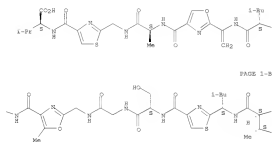
IT 959553-22-6P, (-)-bacillamide C 1020001-70-0P,
 (-)-bacillamide C
 RL 22H (Synthetic preparation) / PREP (Preparation)
 (Synthesis of (-)-bacillamide C via Upi multicomponent reaction using
 A chiral auxiliary)
 NH 959553-22-6 CAPLUS
 CN 4-Thiazolecarboxamide, 2-[(1R)-1-(acetylamino)ethyl]-N-[2-[(1R)-indol-3-yl-ethyl]-] - (CA INDEX NAME)
 Absolute stereochemistry.



NH 1010001-19-0 CAPLUS
 CN 4-Thiazolecarboxamide,
 2-[1-(acetylamino)ethyl]-N-[2-[(1R)-indol-3-yl-ethyl]-]
 (CA INDEX NAME)



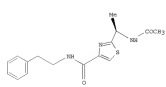
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REFERENCE COUNT: 43 THERE ARE 43 CITED REFERENCES AVAILABLE FOR
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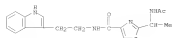
L31 ANSWER 2 OF 53 CAPLUS COPYRIGHT 2010 ACS on STM
 ACCESSION NUMBER: 20091405301 CAPLUS
 DOCUMENT NUMBER: 15219575
 TITLE: Biosynthesis of indolocarbazole and goadsporin, two
 different heterocyclic antibiotics produced by
 actinomycetes
 AUTHOR(S): Ohsaka, Hiroyasu
 CORPORATE SOURCE: Department of Biotechnology, Faculty of Engineering
 and Biotechnology Research Center, Toyama Prefectural
 University, 5260 Gofukue, Imizu, Toyama, 939-0398,
 Japan
 SOURCE: Bioscience, Biotechnology, and Biochemistry (2009),
 77(10), 2149-2155
 CUBIN: BBIJL; ISSN: 0916-4411
 PUBLISHER: Japan Society for Bioscience, Biotechnology, and
 Agrochemistry
 JOURNAL: Journal of General Review
 LANGUAGE: English
 AB: A review. The biosynthesis of staurosporine, eburosporine, and
 goadsporin, which are produced by actinomycetes and contain
 characteristic
 heterocyclic rings, was characterized by genetic methods. Staurosporine
 and eburosporine contain an indolocarbazole ring synthesized from two
 moles of tryptophan, with indolepyruvic acid and chromopyrrole
 acid
 as biosynthetic intermediates. A tetrameric heterocyclic ring synthesizes
 chromopyrrole acid, and cyclohexene 1,4-diol peroxide catalyzes the
 intramolecular C-C coupling and decarboxylation of chromopyrrole acid to form
 the indolocarbazole core. Goadsporin is a thiopeptide containing
 thiazole and oxazole heterocyclic rings. The structural gene gdh
 is ribosomally translated to a goadsporin precursor peptide, and oxazole,
 methylmalonate, and thiazole rings are derived from serine,
 threonine, and cysteine through post-translational modifications. On the
 basis of these knowledge, a wide variety of indolocarbazole and
 goadsporin analogs through the rational gene recombination and disruption
 of these biosynthetic genes were successfully produced.
 IT 603476-91-5P, Goadsporin
 RL 22H (Biological preparation) / RLGL (Biological study) / PREP
 (Preparation)
 (Biosynthesis of indolocarbazole and goadsporin, two different
 heterocyclic antibiotics produced by actinomycetes)
 NH 603476-91-5 CAPLUS
 CN 1-Valine,
 N-[2-[(1S)-1-(acetylamino)ethyl]-5-methyl-4-oxazolyl]carbamoyl]-
 L-valyl-2-[1-aminoethyl]-5-methyl-4-oxazolecarboxyl-1-isoleucyl-2-[(1S)-
 1-amino-3-methylbutyl]-4-thiazolecarboxyl-1-arylglycyl-2-(aminomethyl)-5-
 methyl-4-oxazolecarboxyl-1-isoleucyl-3-(1-aminoethyl)-4-oxazolecarboxyl-1-
 allyl-2-(1-aminoethyl)-4-thiazolecarboxyl-1- (CA INDEX NAME)
 Absolute stereochemistry. Notation 1-5.

See sponge *Pyrosoma* sp.
 Ye, Lu-Lu; Li, Shen-Yu; Peng, Cheng-Sheng; Li,
 Shi-Tong; Gao, Yue-Mei
 Key Laboratory of Microbial Metabolism, School of
 Life
 Science and Biotechnology, Ministry of Education,
 China, Shanghai Jiao Tong University, Shanghai,
 200240, P.R. China
 Helvetica Chimica Acta (2009), 92(3), 607-612
 CUBIN: BBIJL; ISSN: 0010-291X
 Verlag Helvetica Chimica Acta
 Journal
 English
 GI



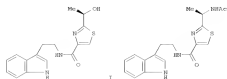
AB A novel thiazole alkaloid, neobacillamide A (1), together with a
 known related one, bacillamide C, was isolated from the bacterium
Bacillus vallismortis CH9, associated with the South China Sea sponge *Pyrosoma*
sp.
 The structure of 1 was elucidated on the basis of its spectroscopic data.
 A plausible biosynthetic pathway is proposed. 1 represents the first
 example of a thiazole-carbamoyl bearing a 2-phenylethylamine
 moiety.
 IT 1158321-83-0P
 RL 102 (Biological study, unclassified) / NBO (Natural product
 occurrence) / PREP (Preparation) / RCP (Reproduction or recovery) / RLGL
 (Biological study) / OCVS (Occurrence) / PREP (Preparation)
 (Neobacillamide A as thiazole-containing alkaloid from marine
Bacillus vallismortis with sponge *Pyrosoma* sp.)
 NH 1158321-83-0 CAPLUS
 CN 4-Thiazolecarboxamide, 2-[(1R)-1-(acetylamino)ethyl]-N-(2-phenylethyl)-
 (CA INDEX NAME)
 Absolute stereochemistry. Notation 1-5.

IN 1050561-79-0 CAPLUS
CN 4-Thiazolecarboxamide,
2-[[1-(acetylamino)ethyl]-N-[2-(1H-indol-3-yl)ethyl]-
-CA INDEX NAME]



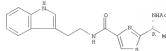
OS CITING REF COUNT: 1 THERE ARE 1 CAPLUS RECORDS THAT CITE THIS RECORD
(1 CITINGS)
REFERENCE COUNT: 8 THERE ARE 8 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RECORD.
FORMAT

L31 ANSWER 6 OF 53 CAPLUS COPYRIGHT 2010 ACS on STM
ACCESSION NUMBER: 20071208407 CAPLUS
DOCUMENT NUMBER: 14914924
TITLE: Bacillides from a hypersaline microbial mat
AUTHOR(S): Socha, Jason M.; Long, Richard A.; Rowley, David C.
CORPORATE SOURCE: Department of Biomedical and Pharmaceutical Sciences,
College of Pharmacy, University of Rhode Island,
Kingston, RI, 02881, USA
SOURCE: Journal of Natural Products (2007), 70(11), 1793-1795
CODEN: JNPEDY; ISSN: 0163-3864
PUBLISHER: American Chemical Society-American Society of Pharmacology
DOCUMENT TYPE: Journal
LANGUAGE: English
OS



AB Chemical studies of a *Bacillus* endophytic isolated from a Bahamian hypersaline microbial mat led to the isolation of bacillides B (I) and C (II), new tryptamide thiazole metabolites. HPLC-guided fractionation using a HPLC-MS/MS bioassay technique enabled the detection of these trace fermentation products, and their total structures were elucidated by combined spectroscopic techniques.
IT 95953-22-49, bacillides C
RI: BSI (Biological study, unclassified); NHO (Natural product occurrence); PEP (Preparation); POF (Purification or recovery); RICH (Biological study); CCS (Concentration); PEP (Preparation)
(Bacillides from a hypersaline microbial mat bacterium)
IN 95953-22-4 CAPLUS
CN 4-Thiazolecarboxamide, 2-[[1-(1-acetylamino)ethyl]-N-[2-(1H-indol-3-yl)ethyl]- -CA INDEX NAME]

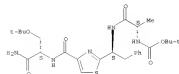
Absolute stereochemistry.



OS CITING REF COUNT: 8 THERE ARE 8 CAPLUS RECORDS THAT CITE THIS RECORD
(8 CITINGS)
REFERENCE COUNT: 15 THERE ARE 15 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RECORD.
FORMAT

L31 ANSWER 7 OF 53 CAPLUS COPYRIGHT 2010 ACS on STM
ACCESSION NUMBER: 20071442008 CAPLUS
DOCUMENT NUMBER: 14773042
TITLE: Peptide-embedded heterocycles by mild single and multiple *aza*-Wittig ring closures
AUTHOR(S): Kiedrich, Matthias; Mach, Andreas; Arnold, Hans-Dieter
CORPORATE SOURCE: Fachbereich Chemis, Universitat Dortmund, Dortmund, 44221, Germany
SOURCE: Angewandte Chemie, International Edition (2007), 46(15), 2701-2705
CODEN: ACHIEF; ISSN: 1433-7851
PUBLISHER: Wiley-VCH Verlag GmbH & Co. KGaA
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 14773042
AB The *aza*-Wittig cyclization of amine acids and peptides is extremely mild, selective, and versatile. The reaction of amine acid esters and amine acid thioesters affords delivered peptide 1,2-succinates and 1,7-succinates with unsaturated functional-group tolerance. This method allowed multiple ring closures and tolerates aqueous solvents.
IT 94051-17-70
RI: BSI (Synthetic preparation); PEP (Preparation)
(Preparation of thiazole-containing peptide via esterification of *tert*-protected dipeptide with azide substituted dipeptide followed by *aza*-Wittig condensation)
IN 94051-17-7 CAPLUS
CN Carbanic acid, N-[[15]-2-[[15]-1-[4-[[15]-2-amino-1-[[1,1-dimethylethoxy)methyl]-2-methoxy]phenyl]carbonyl]-1-thiazolyl]-2-phenylethylamino]-1-methyl-2-methoxy]-, 1,1-dimethylethyl ester [CA INDEX NAME]

Absolute stereochemistry.



OS CITING REF COUNT: 9 THERE ARE 9 CAPLUS RECORDS THAT CITE THIS RECORD
(9 CITINGS)
REFERENCE COUNT: 46 THERE ARE 46 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RECORD.
FORMAT

A3 The biosynthetic gene cluster of trichostatin, a polypeptide antibiotic containing thiazole and oxazole rings, was cloned from *Streptomyces* sp. TP-90164. The cluster contains 1 structural gene, godA, and nine god (godapin) genes involved in post-translational modification, immunity and transcriptional regulation. Although the gene organization is similar.

to typical hemoglobin biosynthetic gene clusters, each gsdoprin biosynthetic gene shows low homology to these genes. Gsdoprin biosynthesis is initiated by the translation of *gsdA*, and the subsequent prenylation, dehydration and acetylation are probably catalyzed by *gsdW*, *gsdU*, *gsdQ* and *gsdS*, respectively. The high similarity to the *hbaA* gene suggests that the signal recognition particle also plays an important role in gsdoprin insertion. Furthermore, four gsdoprin analogs were produced by site-directed mutagenesis of *gsdA*, suggesting that this biosynthetic machinery is used for the heterocyclization of

IT 88459-33-3P
RL: RM (Biosynthetic preparation); PRP (Properties); BIOL (Biological study); PRP (Preparation)
[20K; cloning and characterization of goudsporin biosynthetic gene
region from *Chaetomium* sp. 88459-33-3P]

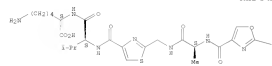
[illegible]

L-valyl-2-(1-aminobutyl)-5-methyl-4-oxazolecarboxyl-L-isoleucyl-2-(18)-

1-amino-3-methylbutyl]-4-thiazolecarbonyl-L-serylglycyl-2-(aminomethyl)-5-methyl-4-oxazolecarbonyl-L-leucyl-2-(1-aminobenzyl)-4-oxazolecarbonyl

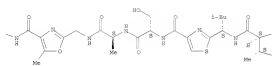
Absolute stereochemistry.

PAGE 1-8

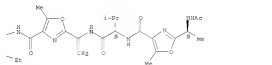


131 ANSWER 8 OF 53 CAPLOS COPYRIGHT 2010 ACS on STM (Cont. invd)

PAGE 1-2



PAGE 1-C



IT 884593-32-2P
 XL: BFN (Biosynthetic preparation); PRP (Properties); BIOL (Biological study); PREP (Preparation)
 (8357); cloning and characterization of gadsaporin biosynthetic gene

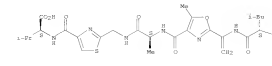
884593-32-2 CAPLOS
L-Valine,

N-[2-[15]-1-(acetylanino)ethyl]-5-methyl-4-oxazolyl carbonyl)-
L-valyl-2-[1-anisoethenyl]-5-methyl-4-oxazolecarbonyl-L-isoleucyl-2-[15]-

1-amino-3-methylbutyl]-4-thiazolecarbonyl-L-serylglycyl-2-(aminomethyl)-5-methyl-4-oxazolecarbonyl-L-leucyl-2-(1-aminooethyl)-5-methyl-4-

oxazolecarbonyl-L-alanyl-2-(aminomethyl)-4-thiazolecarbonyl- (9Cl) (G)
INDEX NAME]

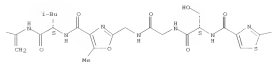
PAGE 1-A



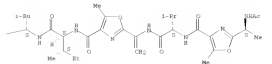
131 ANSWER 8 OF 53 CAPLITE COPYRIGHT 2010 ACS on STM (Continued)

(Cont. on next page)

PAGE 1-2



PAGE 1-C



IT 884593-31-1P
RL: H90 (Biosynthetic preparation); PKP (Properties); BIOL (Biological study); PREP (Preparation)
[GIGA: cloning and characterization of gadsperin biosynthetic gene cluster from *Streptomyces* sp. 10164]

```

cluster from Streptococcus sp. AT-00584)
IN  884593-31-1 CAPLOS
CN  L-Valine,
M  112 11861 3 1-methyl-2-methylbutyl 2-methyl-4-oxo-2-pentenoate

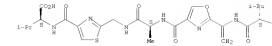
```

L-valyl-2-[(11)-1-[(aceylamino)ethyl]-5-methyl-4-oxazolyl]carboxyl)-

1-amino-3-methylbutyl]-4-thiazolecarbonyl-L-seryl-L-alanyl-2-(aminomethyl)-

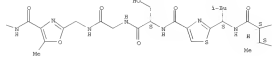
5-methyl-1-4-oxazolecarbonyl-1-L-leucyl-2-[1-anilinoethyl]-4-oxazolecarbonyl-1-L-alanyl-2-(anilinoethyl)-4-thiazolecarbonyl- (9CI) (CA INDEX NAME)

PAGE 1-A

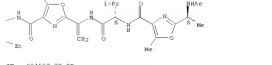


131 ANSWER 8 OF 53 CAPLOS COPYRIGHT 2010 ACS on STM (Continued)

PAGE 1-2



PAGE 1-C



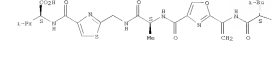
study); PREP (Preparation)
[T55; cloning and characterization of geadsporin biosynthetic gene
cluster from Streptomyces sp. TP-A0584]
884593-30-0 CAPLOS

N-[[2-[(18)-1-(acetylamino)ethyl]-5-methyl-4-oxazoly]carbonyl]-

L-valyl-2-[(1-aminocyclohexyl)-4-oxazolecarbonyl-L-isoleucyl-2-[(1S)-1-amino-3-methylbutyl]-4-thiazolecarbonyl-L-serylglycyl-2-(aminomethyl)-5-methyl-oxazolecarbonyl-L-leucyl-2-[(1-aminocyclohexyl)-4-oxazolecarbonyl-L-alanyl-

Absolute stereochemistry.

PAGE 1-A



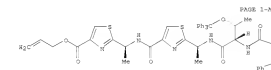
L31 ANMER 9 OF 53 CAPLUS COPYRIGHT 2010 ACS on STN (Continued)
 (2 CITINGS)
 REFERENCE COUNT: 5 THERE ARE 5 CITED REFERENCES AVAILABLE FOR THIS
 RECORD. ALL CITATIONS AVAILABLE IN THE RE
 FORMAT

L31 ANMER 10 OF 53 CAPLUS COPYRIGHT 2010 ACS on STN
 ACCESSION NUMBER: 2005/24364 CAPLUS
 DOCUMENT NUMBER: 142/482299
 TITLE: Total synthesis of didiolanides A and B
 AUTHOR(S): Yoo, Shu-Li; Kelly, Jeffrey M.
 CORPORATE SOURCE: Department of Chemistry, Scripps Institute for
 Chemical
 SOURCE: Biology, Scripps Research Institute, La Jolla, CA,
 92037, USA
 LANGUAGE: Telcelotron Letters (2005), 46(15), 2567-2570
 CODEN: TELACT ISSN: 0040-4039
 KEYWORD: B.V.
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 OTHER SOURCE(S): CASREACT 142/482299
 AB The first total synthesis of didiolanides A and B has been accomplished
 by
 the solid phase assembly of thiazole-containing amino acids and over,
 available from protected (Pac - 3-(isopropylthio)propanoyl) amino
 acids. The synthesis of didiolanide B was also achieved in high yield
 using solution phase peptide synthesis. The thiazole-containing amino
 acid composing didiolanides A and B was synthesized by a NaO_2 oxidation
 of a
 thiazoline, prepared from an Ala-Cys dipeptide using
 Bz (triphenylboron)phosphonium trifluoromethanesulfonate. The final
 macrocyclization was accomplished efficiently by Fmoc and HMP in
 solution.
 ST 851792-99-3P 851791-00-3P
 RE: RCT (Reactant); SRI (Synthetic preparation); PREP (Preparation); RACT
 (Reactant or reagent)
 (Total synthesis of didiolanide B by solution coupling)
 RE 851790-99-3 CAPLUS
 CH 4-Thiazolecarboxylic acid, 2-[(1S)-1-[[[2-[(1S)-3-[[[2S,3S]-2-[[119S]-
 fluoron-9-yl]ethoxy]carbonyl]amino]-1-oxo-3-
 (triphénylmethyl)amino]ethyl]-4-thiazolyl]oxy]amino]ethyl]-,
 2-propen-1-yl ester (CA INDEX NAME)
 Absolute stereochemistry.

L31 ANMER 10 OF 53 CAPLUS COPYRIGHT 2010 ACS on STN (Continued)
 (Continued)
 PAGE 1-B



RE 851791-00-3 CAPLUS
 CH 1-Threoninamide, N-[[[R]-[fluoren-9-ylmethoxy]carbonyl]-L-phenylalanyl]-N-
 [[1S]-1-[[4-[[[1S]-1-[[4-[(2-propenyl)oxy]amino]-1-2-
 thiazolyl]ethyl]amino]ethyl]-2-thiazolyl]ethyl]-O-(triphénylmethyl)-
 (R)-1 (CA INDEX NAME)
 Absolute stereochemistry.



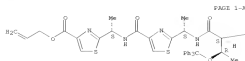
PAGE 1-B



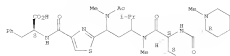
OS-CITING REF COUNT: 14 THERE ARE 14 CAPLUS RECORDS THAT CITE THIS
 RECORD (14 CITINGS)
 REFERENCE COUNT: 26 THERE ARE 26 CITED REFERENCES AVAILABLE FOR
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 RECORD. ALL CITATIONS AVAILABLE IN THE RE
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L31 ANMER 10 OF 53 CAPLUS COPYRIGHT 2010 ACS on STN (Continued)

PAGE 1-A

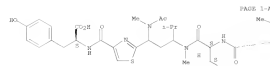


L31 ANMER 12 OF 53 CAPLUS COPYRIGHT 2010 ACS ON STN (Continued)
Absolute stereochemistry.



RN 444961-04-6 CAPLUS
CN 1-Tyrosine, (2R)-2-methyl-2-piperidinecarboxyl-1-isoleucyl-2-[1-(acetylmethylamino)-4-methyl-3-(methylamino)pentyl]-4-thiazolcarboxyl-1- (PC1) (CA INDEX NAME)

Absolute stereochemistry.



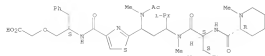
PAGE 1-A



PAGE 1-B

RN 444961-05-7 CAPLUS
CN Acetic acid, 2-[(2R)-2-[[[2-[1-(acetylmethylamino)-4-methyl-3-(methyl-[[2S,3S]-2-methyl-2-[[[2R)-1-methyl-2-piperidinyl]oxycarbonyl]amino]-1-oxopentyl]amino]pentyl]-4-thiazolyl]oxycarbonyl]amino]-3-phenylpropyl]- (CA INDEX NAME)

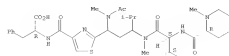
Absolute stereochemistry.



L31 ANMER 12 OF 53 CAPLUS COPYRIGHT 2010 ACS ON STN (Continued)

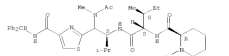
RN 444961-06-8 CAPLUS
CN 2-Phenylalanine, (2R)-3-methyl-2-piperidinecarboxyl-1-isoleucyl-2-[1-(acetylmethylamino)-4-methyl-3-(methylamino)pentyl]-4-thiazolcarboxyl-1- (PC1) (CA INDEX NAME)

Absolute stereochemistry.



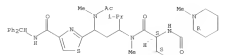
RN 444961-15-9 CAPLUS
CN 2-Piperidinecarboxamide, N-[(1S,2S)-1-[[[1S]-3-[[[acetylmethylamino]-4-[[[diphenylmethyl]amino]carboxyl]-2-thiazolyl]-3-[[[1S]-2-methylpropyl]amino]carboxyl]-2-methylbutyl]-1-methyl-, (2R)- (CA INDEX NAME)

Absolute stereochemistry.



RN 444961-16-2 CAPLUS
CN 2-Piperidinecarboxamide, N-[(1S,2S)-1-[[[1S]-3-[[[acetylmethylamino]-3-[[4-[[[diphenylmethyl]amino]carboxyl]-2-thiazolyl]-3-[[[1S]-2-methylpropyl]amino]carboxyl]-2-methylbutyl]-1-methyl-, (2R)- (CA INDEX NAME)

Absolute stereochemistry.



OS.CITING REF COUNT: 6 THERE ARE 6 CAPLUS RECORDS THAT CITE THIS RECORD (7 CITINGS)
REFERENCE COUNT: 1 THERE ARE 1 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE AS FORMAT

L31 ANMER 12 OF 53 CAPLUS COPYRIGHT 2010 ACS ON STN (Continued)

L31 ANMER 12 OF 53 CAPLUS COPYRIGHT 2010 ACS ON STN (Continued)
2003-013011 CAPLUS
DOCUMENT NUMBER: 140247690
TITLE: Determination of the absolute configuration of thiazole-containing amino acids in a peptide using the advanced Marfey's method
AUTHOR(S): Fujii, Kiyomasa; Nakano, Tomoyo; Imanishi, Shunzo; Harada, Ken-ichi
CORPORATE SOURCE: Faculty of Pharmacy, Meijo University, Japan
SOURCE: Tennen Taki, Nagabutsu Tokonaka, Keen Yoshitaku (2011), Chok, 389-394
CODEN: TPKYDE
PUBLISHER: Nippon Kagakuai
DOCUMENT TYPE: Journal
LANGUAGE: Japanese
AB A symposium report : A large number of peptide containing the modified amino acids such as thiazole (Tz) and oxazole (Ox) rings have been isolated from cyanobacteria and marine origins. In general, the absolute configuration of such a modified amino acid in a peptide is determined on the basis of that of the corresponding intact amino acid derived from the hydrolyzate after chemical treatments. In order to derive intact amino acids from Tz-amino acids in a peptide, Ireland et al. proposed a method composed of acid hydrolysis combined with ozonolysis in 1993. Since then, although this method has been applied to many peptides containing Tz-amino acids, no method has been established for the direct detection and the identification of Tz-amino acids including the absolute configuration. The authors have established a nonempirical method using LC/MS, the advanced Marfey's method, which includes HPLC with a rational guideline, a sensitive derivatizing reagent, FPLA (1-fluoro-2,4-dinitrophenyl-5-isocyanide), and a racemization procedure using DL-FPLA, for determination of the absolute configuration of constituent amino acids and amine in a peptide. Therefore, they considered that Tz-amino acids in the hydrolyzate can be directly detected and determine the absolute configuration by the 'advanced Marfey's method' without ozonolysis. For the determination of the absolute configuration of Tz-amino acids in a peptide, they applied the advanced Marfey's method to the isolated microcycloamide (I) containing two Tz-amino acids. Tz-amino acids could be directly detected together with a constituent amino acid in the hydrolyzate by this method, although they were concealed under ordinary hydrolysis conditions as expected. According to the proposed separation mechanism of Marfey's method, the elution order of Tz-amino acids can be basically determine in the same way as amino acids. In order to identify each original peak of Tz-amino acids, the flash hydrolysis (NH₄Cl, 110°C, 1 h) was introduced for the control of the racemization during the acid hydrolysis.
Consequently, the absolute configuration of I containing Tz-amino acids was clearly determined. Adm., this method with the flash hydrolysis was successfully applied to

131 ARMERIA 13 OF 53 CAPLUS COPYRIGHT 2010 ACS on STM (Continued)
the detn. of the abs. configuration of constituent amino acids in two
naturally occurring peptides, wasakamide and goadsporin, possessing
7A-amino acids. The methodol. using LC/MS combined with flash hydrolysis
is being further extended for the structural detn. of various naturally
occurring peptides possessing the modified amino acids and D-amino acids.
1T 403476-91-5, Goadsporin

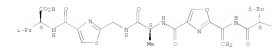
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(determinant) of the absolute configuration of thiazole-containing
amino acids in a peptide using the advanced Marfey's method)
PEI 401474-91-8 CAS/55
CI 1-Valine,
SI [[-115]-1-(acetylamino)ethyl]-5-methyl-4-oxazolinyl]carbonyl]-
1-Valyl]-2-[1-aminoethyl]-5-methyl-4-oxazolinyl]-2-[1S]-
1-amino-3-methylthyl]-4-thiazolecarboxyl]-1-serinyl]-2-[1-aminoethyl]-5-
methyl-4-oxazolinyl]-1-Valyl]-2-[1-aminoethyl]-4-oxazolinyl]-1-
alanyl]-2-[1-aminoethyl]-4-thiazolecarboxyl]- (CA INDEX NAME)

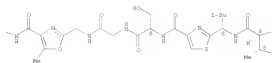
Absolute stereochemistry. Notation (-).

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PAGE 1-A

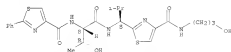


PAGE 1-2



133 ANHWA 14 OF 15 CAPSUS COPYRIGHT 2010 ACS ON 978
 134 200912131
 135 1391294515
 136
 137 Structure-based design of agents targeting the
 138 bacterial ribosome
 139
 140 Sower, Thiruv; Drysdale, Martin; Isomson, Richard;
 141 Sower, Alan; Leach, Andrew; Maitland, Robert;
 142 Sower, Alan; Leach, Andrew; Maitland, Robert;
 143 Murchie, Alistair; Powles, Jennifer; Houghley, Stephen
 144 Department of Medicinal Chemistry, Kilmoragh Hall,
 145 University of Central England, Birmingham, B4 7ET,
 146 Birmingham, UK
 147 Broomfield & Medical Chemical Letters (2003),
 148 1(1), 245-248
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 150 ORCID: BMCL; Email: SCS: 0940-284X
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Absolute stereochemistry.

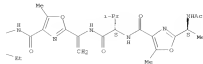


F20 666235-50-3 CAPSULE
 C01 4-Thiazolecarboxamide, N-[[[(1S,2R)-1-[[[(1S)-2-[4-[[[1,3-benzodioxol-5-ylmethyl]amino]carbonyl]-2-thiazolyl]propyl]amino]carbonyl]-2-hydroxypropyl]-2-methyl- (CA INDEX NAME)

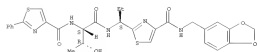
Absolute stereochemistry

L21 ANSWER 11 OF 51 CAPLOS COPYRIGHT 2019 ACS on STN (Continued)

PAGE 1-C



L31 ANSWER 14 OF 53 CAPLOS COPYRIGHT 2010 ACS on STN (Continued)

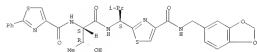


```

NN 666235-51-4 CAMPUS
CN 4-Thiazolecarboxamide, N-[[(1S,2R)-1-[[[[(1S)-1-[4-[[[1,3-benzodioxol-5-ylmethyl]amino]carbonyl]-2-thiazolyl]-2-methylpropyl]amino]carbonyl]-2-hydroxypropyl]-2-phenyl]- (CA INDEX NAME)

```

Absolute stereochemistry

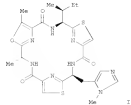


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08..CITING REF COUNT: 18  THERE ARE 18 CAPLUS RECORDS THAT CITE THIS
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REFERENCE COUNT: 18      THERE ARE 18 CITED REFERENCES AVAILABLE FOR
THIS                     RECORD. ALL CITATIONS AVAILABLE IN THE RE
FORMAT

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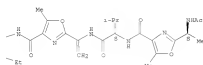
L31 ANMER 15 OF 53 CAPLUS COPYRIGHT 2010 ACS ON STN
 ACCESSION NUMBER: 2002;641298 CAPLUS
 DOCUMENT NUMBER: 15919527
 TITLE:
 Simultaneous detection and determination of the absolute configuration of thiazole-containing amino acids in a peptide
 AUTHOR(S): Fujii, Kiyonaga; Yabashi, Yukio; Nakano, Tomoyo; Imachi, Shunzo; Iwata, Susane F.; Harada, Ken-ichi
 CORPORATE SOURCE: Faculty of Pharmacy, Meijo University, Tempaku, Nagoya, 468-8502, Jpn
 SOURCE: Tetrahedron (2002), 58(34), 6873-6879
 COUNTRY: JAPAN; ISSN: 0040-4039
 PUBLISHER: Elsevier Science Ltd.
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 GI



AB For the simultaneous detection and determination of the absolute configuration of a thiazole-containing (Trl-) amino acid in a peptide, we have developed a reliable method using the 'advanced Marfey's method', which includes HPLC with a rational epimerase, a sensitive derivatizing reagent, 1-fluoro-2,4-dinitrophenyl-5-L-leucanilamide (D-FDLA), and a racemization procedure using D-FDLA for determination of the absolute configuration of essential amino acids in a peptide. Trl-amino acids could be directly detected in the hydrolysate by this method, although they were racemized under ordinary hydrolysis conditions. In order to depress the racemization, the flash hydrolysis was introduced. As a result, the flash hydrolysis for 1 h was sufficient to detect each constituent amino acid, and it was possible to identify the original peak. Consequently, the absolute configuration of noncyclopeptide 1 possessing Trl-amino acids was determined by the advanced Marfey's method combined with flash hydrolysis. At 13.7 and 24.6 mg/mL (CDCl₃) 1 showed a cytotoxicity against the lymphocytic mouse leukemia and showed an antibacterial activity against *Amoeba* sp. Additionally, this method was successfully applied to the simultaneous detection and determination of the absolute configuration of two other naturally occurring

L31 ANMER 15 OF 53 CAPLUS COPYRIGHT 2010 ACS ON STN (Continued)

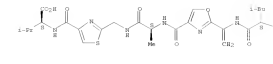
PAGE 1-C



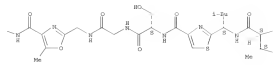
ON-CITING REF COUNT: 13 THERE ARE 13 CAPLUS RECORDS THAT CITE THIS RECORD (13 CITINGS)
 REFERENCE COUNT: 29 THERE ARE 29 CITED REFERENCES AVAILABLE FOR THIS RECORD.
 FORMAT: RECORD. ALL CITATIONS AVAILABLE IN THE PE

L31 ANMER 15 OF 53 CAPLUS COPYRIGHT 2010 ACS ON STN (Continued)
 peptides, malakaloids and gadopidins. The established method with the flash hydrolysis had an added advantage as that labile amino acids, such as tryptophan and methionine sulfoxide, during acid hydrolysis can be detected in the intact form.
 IT 602476-91-5 Gadopidins
 RI: AMT (Analytic); PEP (Preparation); KCT (Reactant); AMST (Analytical study); KCT (Reactant or reagent)
 (detection and determination of absolute configuration of thiazole-containing amino acids in naturally occurring peptides malakaloids and gadopidins)
 RI 602476-91-5 CAPLUS
 CN 1-Valine
 N-[12-(115)-1-(acetylamino)ethyl]-5-methyl-4-oxazolyloxy-2-[(110)-L-valyl]-2-(1-aminomethyl)-5-methyl-4-oxazolocarbonyl-L-isoleucyl-2-[(110)-L-3-amino-3-methylbutyl]-4-thiazolocarboxyl-L-erythylglycyl-2-(1-aminomethyl)-5-methyl-4-oxazolocarbonyl-L-leucyl-2-(1-aminomethyl)-4-oxazolocarbonyl-L-alanyl-2-(1-aminomethyl)-4-thiazolocarboxyl-L- (CA INDEX NAME)
 Absolute stereochemistry. Isotopes 1-7.

PAGE 1-A



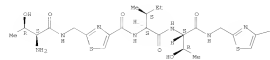
PAGE 1-B



L31 ANMER 16 OF 53 CAPLUS COPYRIGHT 2010 ACS ON STN
 ACCESSION NUMBER: 2002;390798 CAPLUS
 DOCUMENT NUMBER: 13747443
 TITLE:
 Synthesis and structural properties of patellamide A derivatives and their copper(II) compounds
 AUTHOR(S): Bernhardt, Paul V.; Giese, Peter; Fairlie, David P.; Gahan, Lawrence S.; Hanson, Graeme S.; Lotzbeyer, Department of Chemistry, The University of Queensland,
 CORPORATE SOURCE: Brisbane, 4072, Australia
 SOURCE: Chemistry-A European Journal (2002), 8(7), 1517-1536
 COUNTRY: GERMANY; ISSN: 0947-4539
 PUBLISHER: Wiley-VCH Verlag GmbH
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 OTHER SOURCE(S): 13747443
 AB The synthesis, characterization and Cu(II) coordination chemical of three new cyclic peptide ligands, PatJ1 (cyclic-[Ile-Thr-(Gly)Thr-Ile-Thr-(Gly)Thr]), PatJ2 (cyclic-[Ile-Thr-(Gly)Thr-(D)-Ile-Thr-(Gly)Thr]), and PatL (cyclic-[Ile-Ser-(Gly)Thr-Ile-Ser-(Gly)Thr]) are reported. All of these cyclic peptides and their copper(II) compounds are derivatives of patellamide A and have a [24]azacrown-9 macrocyclic structure. All four synthetic cyclic peptides have two thiazole rings but, in contrast to patellamide A, no oxazoline rings. The mol. structure of PatJ, determined by x-ray crystallog., has a saddle conformation with two close-to-parallel thiazole rings, very similar to the geometry of patellamide A. The two coordination sites of PatJ with thiazole-N and amide-N donors are each well preorganized for transition metal ion binding. The coordination of Cu(II) was monitored by UV/vis spectroscopy, and this reveals various (metalatable) mono- and dinuclear Cu(II) complexes whose stoichiometry was confirmed by mass spectra. Two types of dinuclear Cu(II) complexes, [Cu₂(L4)(OEt₂)₂ (n = 6, 8) and [Cu₂(L1L)(OEt₂)₂ (n = 4, 6; L = PatL, PatJ, PatJ2), were identified and analyzed structurally by EPR spectroscopy and a combination of spectra simulations and mol. mechanics calcs. (MM-EPR). The four structures are similar to each other and have a saddle conformation, i.e., derived from the crystal structure of PatJ by a twist of the two thiazole rings. The small but distinct structural differences were characterized by the EPR simulations.

IT 479585-32-39
 RI: KCT (Reactant); RRU (Synthetic preparation); PEP (Preparation); RACT (Reactant or reagent)
 (For preparation of cyclic peptide analog of patellamide A)
 CN 479585-32-9 CAPLUS
 CN 1-isoleucine
 L-threonyl-2-(1-aminomethyl)-4-thiazolocarboxyl-L-isoleucyl-1-threonyl-2-(1-aminomethyl)-4-thiazolocarboxyl-L- (CA INDEX NAME)
 Absolute stereochemistry.

PAGE 1-A



PAGE 1-B



ON-CITING REF COUNT: 21 THERE ARE 21 CAPLUS RECORDS THAT CITE THIS RECORD (3 CITINGS)

REFERENCE COUNT: 45 THERE ARE 45 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RECORD.

FORMAT

ACCESSION NUMBER: 2002:289497 CAPLUS

DOCUMENT NUMBER: 137:20592

TITLE: Cyclic octapeptides containing thiazole.

Effect of stereochemistry and degree of flexibility

on

calcium binding properties.

AUTHOR(S): Chasak, Rodney M.; Gonsky, Robert Fairlie, David

P.; Gahan, Lawrence F.; Hanson, George F.

CHEMISTRY DEPARTMENT, THE UNIVERSITY OF QUEENSLAND,

ST. LOUIS, 6071, Australia

JOURNAL OF THE CHEMICAL SOCIETY, PERKIN TRANSACTIONS

2

[1992], 17, 55-567

CODEN: JCSCJG; ISSN: 1472-779X

PUBLISHER: Royal Society of Chemistry

JOURNAL

LANGUAGE: English

OTHER SOURCE(S): CORDATE 137:20592

AB: Solution conformation and calcium binding properties have been

investigated for the two cyclic octapeptides, cyclo-[D-Thr-D-Val(Thi)-Ile-D (I)

and cyclo-[Thr-Gly-Thi-Ile-Thr-Gly(Thi)-Ile-D (II)] and the results are

compared to those for the cyclic octapeptides previously studied;

acidic residues (III), glutamyl-D (IV), cyclo-[Thr-D-Val(Thi)-Ile-D (V)

and cyclo-[Thr-D-Val-Val-Ile-D (VI)]. Both I and II contain

two heterocyclic thiazole ring constraints but the latter has a

larger degree of flexibility as a consequence of the glycine residues

within the cyclic framework. The solution conformation of I and II was

determined from IR NMR spectra and found to be a 'twisted figure of eight' similar

to that for IV. Complexation studies using IR NMR and CD spectroscopy

yielded 1:1 calcium-peptide binding constants (logK) for the two peptides

[5.3 (I) and 5.7 (II)]. For II the magnitude of the binding constant was

verified by a competition titration using CD. The different

calcium-binding affinities of V (logK = 4.0) and I is attributed to the steric hindrance of

the thiosine residue. The magnitude of the binding constant for II

compared to V and I (all peptides containing two thiazole ring constraints)

demonstrates that the increase in flexibility of the cyclic peptide has a

dramatic effect on the Ca²⁺ binding ability. The affinity for Ca²⁺ thus

decreases in the order (VI) > (V) > (I) > (II) > (I).

The number of carbonyl donors available on each peptide has only a limited effect on

calcium binding. The most important factor is the flexibility, which

allows for a conformation of the peptide capable of binding calcium

efficiently.

IT 43435-12-4P

R1: RCT (Reactant); RNM (Synthetic Preparation); PREP (Preparation); RACT

(Reactant or reagent)

[Preparation, conformation, and calcium-binding properties of two

synthetic

cyclooctapeptides compared to sea squirt cyclooctapeptides]

NM 43435-12-4 CAPLUS

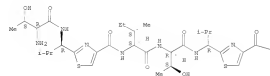
CN 1-isoleucine, D-threonyl-2-[(1R)-1-amino-2-methylpropyl]-4-

thiazolecarboxyl-1-isoleucyl-D-threonyl-2-[(1R)-1-amino-2-methylpropyl]-4-

thiazolecarboxyl-1- [PCI] (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A



PAGE 1-B



ON-CITING REF COUNT: 7 THERE ARE 7 CAPLUS RECORDS THAT CITE THIS RECORD (7 CITINGS)

REFERENCE COUNT: 42 THERE ARE 42 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RECORD.

FORMAT

ACCESSION NUMBER: 2002:11559 CAPLUS

DOCUMENT NUMBER: 136:263447

TITLE: Gadoposin, a chemical substance which promotes

secondary metabolism and morphogenesis in

streptomyces. II. Structure determination

Igarashi, Naohiko; Kan, Yukio; Fujii, Kiyonaga;

Fujita, Tetsuo; Harada, Ken-ichi; Machi, Rieko;

Tabata, Hiroaki; Onaka, Hirojima; Furumai, Tamotsu;

Biotechnology Research Center, Toyama Prefectural

University, Toyama, 939-8599, Japan

JOURNAL OF ANTIMICROBIAL CHEMOTHERAPY, 15(12), 1043-1053

CODEN: JACMAY; ISSN: 0958-0609

PUBLISHER: Japan Antibiotic Research Association

JOURNAL

LANGUAGE: English

AB: The structure of gadoposin was determined by using spectroscopic

techniques.

NMR anal. revealed that gadoposin consists of 19 amino acids, two of

which are dehydroalanines (Deala), and six of which are cyclized to

oxazoles (Ox) and thiazoles (Thi) by dehydrative cyclization

and dehydrogenation from serine, threonine and cysteine. NMR anal.

established seven partial structures, and their sequence was determined

by

CID-MS/MS. Neg. mode FAB-MS/MS gave product ions arising from

charge-remote fragmentation that allowed determination of the sequence of the

amino acid components as H₂N-L-Deala-MeOx-Val-Deala-MeOx-Ile-Leu-Thi-De-

Gly-Gly-MeOx-De-Deala-Ox-L-Ala-Gly-Thi-Val-OH. The chiral amino acids

were determined by the advanced Marfey's method to have L-configurations.

IT 43416-21-3, Gadoposin

R1: PREP (Preparation); RCT (Reactant); RACT (Reactant or reagent)

[Structure determination of the antibiotic gadoposin using NMR and

CID-MS/MS]

NM 43416-21-3 CAPLUS

CN L-Valine,

N-[(2-[(1S)-1-(acetylamino)ethyl]-5-methyl-4-oxazolidinyl)carboxyl]-

L-valyl-2-[(1-aminomethyl)-5-methyl-4-oxazolidinyl]-L-isoleucyl-2-[(1S)-

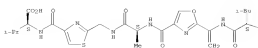
L-amino-3-methylbutyl]-4-(thiazolecarboxyl)-L-erythryl-2-[(1-aminomethyl)-5-

methyl-4-oxazolidinyl]-L-isoleucyl-2-[(1-aminomethyl)-4-oxazolidinyl]-L-

alanine-2-(aminomethyl)-4-(thiazolecarboxyl)- (CA INDEX NAME)

Absolute stereochemistry. Notation (-).

PAGE 1-A



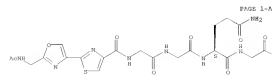
*** STRUCTURE DIAGRAM IS NOT AVAILABLE ***
 NO 254125-18-3 CAPUS
 CH L-1-isoecine, L-valylglycyl-L-
 isoecineylglycylglycylglycylglycylglycylglycylglycyl-2-[2-
 (aminomethyl)-4-thiazolecarboxyl-L-lysyl-L-
 glutamylglycylglycylglycylglycylglycyl-L-4-thiazolecarboxylglycyl-2-
 (aminomethyl)-4-thiazolecarboxyl-L-lysyl-L-
 asparagylglycylglycylglycylglycylglycyl-L-asparagylglycyl-2-
 (aminomethyl)-4-thiazolecarboxylglycyl-2-(aminomethyl)-4-
 oxazolecarboxylglycyl-L-lysyl-L-histidyl- (PCI) (CA INDEX NAME)
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 OS CITING REF CONTRA 20 THERE ARE 20 CAPUS RECORDS THAT CITE THIS
 RECORD (10 CITED)
 REFERENCE CONTRA 27 THERE ARE 27 CITED REFERENCES AVAILABLE FOR
 THIS
 RECORD. ALL CITATIONS AVAILABLE IN THE EE
 FORMAT

L31 ANMER 20 OF 53 CAPUS COPYRIGHT 2010 ACS ON STN
 ACCESSION NUMBER: 2000-900912 CAPUS
 DOCUMENT NUMBER: 131470215
 TITLE: Avirulent brucella with mutated Bacth gene and its
 use
 INVENTOR(S): AL VACCINES
 Levier, Kraling, Walker, Graham C.; Koop, Roy M., II;
 Phillips, Robert M.; Robertson, Gregory T.
 PATENT ASSIGNEE(S): Massachusetts Institute of Technology, USA
 SOURCE: PCT Int. Appl., 27 pp.
 CORRE: FIGURE
 DOCUMENT TYPE: Patent
 LANGUAGE: English
 FAMILY ACC. NUM. COMM: 1
 PATENT INFORMATION:
 PATENT NO. KIND DATE APPLICATION NO. DATE
 WO 200007713 A2 20001211 WO 2000-001549 20000609
 WO 200007713 A3 20010905
 WI, AU, AM, AT, BG, BR, CA, CH, CN, CZ, DE, DK, EE, ES, FI, GB, GR, HU, IE, IL, IN, JP, KR, MA, ME, NL, NO, NZ, PL, PT, RU, SE, SG, SI, SK, SL, TH, TM, TR, TT, UA, US, VE, VN, YU, ZA, ZW
 ME: GB, CH, DE, ES, FI, FR, GB, GR, HU, IE, IL, IN, JP, KR, MA, ME, NL, NO, NZ, PL, PT, RU, SE, SG, SI, SK, SL, TH, TM, TR, TT, UA, US, VE, VN, YU, ZA, ZW
 CT, CY, CZ, DE, ES, FI, FR, GB, GR, HU, IE, IL, IN, JP, KR, MA, ME, NL, NO, NZ, PL, PT, RU, SE, SG, SI, SK, SL, TH, TM, TR, TT, UA, US, VE, VN, YU, ZA, ZW
 PRIORITY APPL. INFO.: OS 1999-138151 P 19990611

AB The present invention discloses a novel approach to attenuating bacteria and their use as live vaccines. In particular, there is disclosed a method of attenuating bacteria Brucella (B.) abortus by mutating Bacth gene, which encodes a membrane protein. The amino acid alignment of Bacth from B. abortus, the Bacth homolog of E. coli, and Bacth from E. coli are provided. The invention also relates to constructing Bacth gene expression vector and mutagenesis of Bacth gene for preparation avirulent Brucella strain used as vaccines. The invention also discloses methods of deliver coops. Into cells by Bacth mediated transport and drug screening methods by identifying Bacth ligands.
 IT B43N-35-2, Microcin B.L
 RI: AGC (Analytical reagent use); AHP (Analytical study); UHS (Uses) (antibiotic) avirulent brucella with mutated Bacth gene and use as vaccines
 BR 8426-90-9 CAPUS
 CH L-1-isoecine, L-valylglycyl-L-
 isoecineylglycylglycylglycylglycylglycylglycylglycylglycyl-2-[2-
 (aminomethyl)-4-thiazolecarboxylglycylglycylglycylglycyl-L-
 glutamylglycylglycyl-2-(aminomethyl)-4-thiazolecarboxylglycyl-2-
 (aminomethyl)-4-thiazolecarboxyl-L-lysyl-L-asparagyl-2-[2-(aminomethyl)-
 4-thiazolecarboxylglycylglycylglycylglycyl-L-asparagylglycyl-2-
 (aminomethyl)-4-thiazolecarboxylglycyl-2-(aminomethyl)-4-
 oxazolecarboxylglycyl-L-lysyl-L-histidyl- (CA INDEX NAME)

*** STRUCTURE DIAGRAM IS NOT AVAILABLE ***
 L31 ANMER 21 OF 53 CAPUS COPYRIGHT 2010 ACS ON STN (Continued)
 ACCESSION NUMBER: 2000-900912 CAPUS
 DOCUMENT NUMBER: 131470215
 TITLE: Bacth, synthesis, and antibacterial activity of a
 peptidomimetic library
 INVENTOR(S): BR, Bi-Huang Martin, Lenore M.
 PATENT ASSIGNEE(S): Department of Biomedical Sciences, College of
 Pharmacy, University of Rhode Island, Kingston, RI,
 02881-0809, USA
 SOURCE: Peptides for the New Millennium, Proceedings of the
 American Peptide Symposium, 18th, Minneapolis, MN,
 United States, June 24-July 1, 1999 (2000), Meeting
 Date 1999, 745-747, Scitex/Int. Fields, Group 2, J.
 Tan,
 Publishers: James P. J. Bramey, George. Kluwer Academic
 Bredrecht, Meth.
 CORRE: 69ATEN
 CONFERENCE
 DOCUMENT TYPE: Conference
 LANGUAGE: English
 AB A symposium report. Building blocks 2-(Fmoc-aminomethyl)thiazole
 4-carboxylic acid (A), 2-(Fmoc-aminomethyl)thiazole 4-carboxylic acid
 and 2-[2'-(Fmoc-aminomethyl)thiazole-4'-yl]thiazole 4-carboxylic
 acid (C) (Fmoc = fluorenylmethoxycarbonyl) were prepared and applied to
 the synthesis of a library of peptidomimetics. Ac-C-G-3-NH(CH2)2NH2,
 Ac-C-G-3-NH(CH2)2NH2, and Ac-C-G-3-NH(CH2)2NH2 were assayed for
 antibacterial activity.
 IT 27115-25-60
 RI: BAC (Biological activity or effector, except adverse); BEO
 (Biological study, unclassified); SPN (Synthetic preparation); BEO (Biological study); PREP (Preparation) (design, synthesis, and antibacterial activity of peptidomimetic library)
 BR 27115-25-60 CAPUS
 CH Glycinamide, N-[[2-[2-(acetaminomethyl)-4-oxazolyl]-4-
 thiazolyl]carboxylglycylglycyl-L-glutamylglycylglycyl-2-(aminomethyl)-4-
 thiazolecarboxyl- (PCI) (CA INDEX NAME)
 Absolute stereochemistry.

L31 ANMER 21 OF 53 CAPUS COPYRIGHT 2010 ACS ON STN
 ACCESSION NUMBER: 2000-900912 CAPUS
 DOCUMENT NUMBER: 131470215
 TITLE: Bacth, synthesis, and antibacterial activity of a
 peptidomimetic library
 INVENTOR(S): BR, Bi-Huang Martin, Lenore M.
 PATENT ASSIGNEE(S): Department of Biomedical Sciences, College of
 Pharmacy, University of Rhode Island, Kingston, RI,
 02881-0809, USA
 SOURCE: Peptides for the New Millennium, Proceedings of the
 American Peptide Symposium, 18th, Minneapolis, MN,
 United States, June 24-July 1, 1999 (2000), Meeting
 Date 1999, 745-747, Scitex/Int. Fields, Group 2, J.
 Tan,
 Publishers: James P. J. Bramey, George. Kluwer Academic
 Bredrecht, Meth.
 CORRE: 69ATEN
 CONFERENCE
 DOCUMENT TYPE: Conference
 LANGUAGE: English
 AB A symposium report. Building blocks 2-(Fmoc-aminomethyl)thiazole
 4-carboxylic acid (A), 2-(Fmoc-aminomethyl)thiazole 4-carboxylic acid
 and 2-[2'-(Fmoc-aminomethyl)thiazole-4'-yl]thiazole 4-carboxylic
 acid (C) (Fmoc = fluorenylmethoxycarbonyl) were prepared and applied to
 the synthesis of a library of peptidomimetics. Ac-C-G-3-NH(CH2)2NH2,
 Ac-C-G-3-NH(CH2)2NH2, and Ac-C-G-3-NH(CH2)2NH2 were assayed for
 antibacterial activity.
 IT 27115-25-60
 RI: BAC (Biological activity or effector, except adverse); BEO
 (Biological study, unclassified); SPN (Synthetic preparation); BEO (Biological study); PREP (Preparation) (design, synthesis, and antibacterial activity of peptidomimetic library)
 BR 27115-25-60 CAPUS
 CH Glycinamide, N-[[2-[2-(acetaminomethyl)-4-oxazolyl]-4-
 thiazolyl]carboxylglycylglycyl-L-glutamylglycylglycyl-2-(aminomethyl)-4-
 thiazolecarboxyl- (PCI) (CA INDEX NAME)
 Absolute stereochemistry.



PAGE 1-A

PAGE 1-B



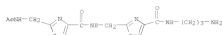
PAGE 1-B

—(CH2)3—NH2

297165-53-0 CAPLOS
4-Thiazolecarboxamide, 2-[[[2-[[[acetyl(amino)methyl]-4-thiazolyl]carbonyl]amino]methyl]-8-[3-aminopropyl]- (CA INDEX NAME)



297165-55-0 CAPLOS
4-Oxazolecarboxamide, 2-[[[2-[[[acetyl(amino)methyl]-4-thiazolyl]carbonyl]amino]methyl]-8-[3-aminopropyl]- (CA INDEX NAME)



297165-51-2 CAPLOS
4-Thiazolecarboxamide, 2-[[[2-[[[acetyl(amino)methyl]-4-thiazolyl]carbonyl]amino]methyl]-8-[4-[[[3-aminopropyl]amino]carbonyl]-2-thiazolyl]methyl]- (PCT) (CA INDEX NAME)

PAGE 1-A



L31 ANMER 23 OF 53 CAPLOS COPYRIGHT 2010 ACS ON STM
ACCESSION NUMBER: 2009:61335 CAPLOS
DOCUMENT NUMBER: 133132166
TITLE: Lanthiobioses and microcins. Polypeptides with unusual chemical diversity
AUTHOR(S): Jody, Ralph W.; Jody, Gunther
CORPORATE SOURCE: Institut für Organische Chemie, der Universität
Tübingen, Tübingen, 72076, Germany
SOURCE: Current Opinions in Chemical Biology (2000), 4(3), 310-317
PUBLISHER: Elsevier Science Ltd.
DOCUMENT TYPE: Journal; General Review
LANGUAGE: English
AB: A review with 58 refs. is given. Bacterial-derived antimicrobial polypeptides enjoy a large degree of structural and chemical diversity.

2 Well-studied examples of such polypeptides are the lantibiotics-containing lantibiotics produced by a variety of gram-pos. bacteria, and their derivatives. Currently, the microcins. Both groups are produced as gene-encoded precursor peptides and undergo post-translational modification to generate the active molecules. Structure elucidation of novel lantibiotics and microcins has recently uncovered further novel structural and chemical features and, combined with the generation of analog peptides by genetic manipulation, new insights into structure-function relationships were gained. Furthermore, study of the mode of action of the lantibiotics nisin and nisinamide has revealed their use of a "docking mol." in the target cell to facilitate their biol. activities.

Meanwhile, in vitro studies with microcin B17 have helped to uncover the mol. mechanisms by which post-translational modification results in the formation of heterocyclic oxazole and thiazole rings. Both groups of polypeptides represent new lead structures for future development of antimicrobial agents, while the identification of the "docking mol." represents a step forward in the search for novel targets for future antibiotics.

IT 8418-30-8, Microcin B17
BI: BC (Biological activity or effector, except adverbs) / BPP (Biological processes) / BPP (Biological study, unclassified) / BPP (Properties) / B10L (Biological study) / PPOC (Processes)
STRUCTURE, Unpublished, and activity of microcins

297165-50-8 CAPLOS
4-Thiazolecarboxamide, 2-[[[2-[[[acetyl(amino)methyl]-4-thiazolyl]carbonyl]amino]methyl]-8-[4-[[[3-aminopropyl]amino]carbonyl]-2-thiazolyl]methyl]- (CA INDEX NAME)

*** STRUCTURE DIAGRAM IS NOT AVAILABLE ***
ON CITING REF COUNT: 91 THERE ARE 91 CAPLOS RECORDS THAT CITE THIS RECORD (91 CITINGS)
REFERENCE COUNT: 58 THERE ARE 58 CITED REFERENCES AVAILABLE FOR THIS

—CH2—NH2

ON CITING REF COUNT: 2 THERE ARE 2 CAPLOS RECORDS THAT CITE THIS RECORD
(2 CITINGS)
REFERENCE COUNT: 0 THERE ARE 0 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE SE
FORMAT

L31 ANMER 23 OF 53 CAPLOS COPYRIGHT 2010 ACS ON STM (Continued)
ON CITING REF COUNT: 2 THERE ARE 2 CAPLOS RECORDS THAT CITE THIS RECORD. ALL CITATIONS AVAILABLE IN THE SE
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*** STRUCTURE DIAGRAM IS NOT AVAILABLE ***
RN  234125-17-8  CAPLOS
CN  L-Isoleucine, L-valylglycyl-L-

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REFERENCE COUNT: 39 THERE ARE 39 CITED REFERENCES AVAILABLE FOR
THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE
FORMAT

CELLS fitted partial atomic charges.
 IT 223680-45-3 223680-49-7
 KL: PEP (Physicoal., engineering or chemical process); PROC (Process)
 (ab initio) calcs. on peptide-derived oxazoles and thiazoles
 NN 223680-45-3 CAPSUS
 CN 4-Thiazolecarboxamide, 2-[(1R)-1-(acetylamino)ethyl]-N-[(1R)-2-amino-1-methyl-2-oxoethyl]- (CA INDEX NAME)



REFERENCE COUNT: 44 THERE ARE 44 CITED REFERENCES AVAILABLE FOR
THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE
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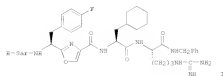
L31 ANMERK 31 OF 53 CAPLUS COPYRIGHT 2010 ACS ON STM
 ACCESSION NUMBER: 1999:120221 CAPLUS
 DOCUMENT NUMBER: 129:299581
 ORIGINAL REFERENCE NO.: 129:61017a,61020a
 TITLE: Thiazole and oxazole peptides: biosynthesis and molecular machinery
 AUTHOR(S): Roy, Sankar; Saha, Debajyoti, Amy M.; Malm, Jill C.; Balshaw, Peter J.; Walsh, Christopher T.
 DEPARTMENT OF BIOLOGICAL CHEMISTRY AND MOLECULAR PHARMACOLOGY, HARVARD MEDICAL SCHOOL, BOSTON, MA, 02115, USA
 SOURCE: Natural Product Reports (1999), 16(12), 249-263
 CODEN: NPRT-PP; ISSN: 0263-4558
 PUBLISHER: Royal Society of Chemistry
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 AB: A review, with 124 refs., Among the enzymic post-translational modifications of peptides, natural products are heterocyclizations of serine, threonine, and cysteine side chains onto the preceding carbonyl group to create five ring heterocycles in the oxazole and thiazole series. Initial products of cyclodehydration are the α -hydroxyketone, and thiazole and oxazole rings are formed under reductive change. A two-electron oxidation generates the heteroatom, oxazole and thiazole systems, which are then cyclized to the five-membered double bonds would create the thiazolidine and oxazolidine rings. All three oxidation states are seen in natural products. The heterocyclizations not only alter peptide backbone connectivity and electronic distribution but also afford new recognition elements for interaction with such targets as DNA and RNA and with proteins that effect the specific final readouts of these natural products.
 IT 8426-90-5, Microcin B7
 RI: B7N (Biological study, unclassified); NFM (Metabolic formation); PKP (Preparative); B7O (Biological study); FOM (Formation, nonpreparative)
 NO 8426-90-5 CAPLUS
 CH 1-Isocysteine, L-valylglycyl-L-isoleucylglycylglycylglycylglycylglycylglycylglycyl-L-[2-(aminomethyl)-4-oxazolidinonylglycyl]-2-(aminomethyl)-4-oxazolidinonylglycyl-L-glutamylglycylglycyl-L-[2-(aminomethyl)-4-thiazolidinonylglycyl]-L-argyl-L-asparagyl-L-[2-(aminomethyl)-4-thiazolidinonylglycyl]-L-argyl-L-asparagylglycyl-L-[2-(aminomethyl)-4-oxazolidinonylglycyl]-2-(aminomethyl)-4-oxazolidinonylglycyl-L-argyl-L-asparagylglycyl-L-[2-(aminomethyl)-4-thiazolidinonylglycyl]-L-argyl-L-asparagylglycyl-L-CA INDEX NAME
 *** STRUCTURE DIAGRAM IS NOT AVAILABLE ***
 OC-CITING REF COUNT: 119 THERE ARE 119 CAPLUS RECORDS THAT CITE THIS RECORD (110 CITINRES)
 REFERENCE COUNT: 124 THERE ARE 124 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L31 ANMERK 32 OF 53 CAPLUS COPYRIGHT 2010 ACS ON STM
 ACCESSION NUMBER: 1998:572745 CAPLUS
 DOCUMENT NUMBER: 129:299581
 ORIGINAL REFERENCE NO.: 129:61017a,61020a
 TITLE: Replacement of thiazole ring formation by the peptide-heterocyclizing microcin B7 Synthetase Using High-Resolution MS/MS
 AUTHOR(S): Kelleher, Neil L.; Balshaw, Peter J.; Walsh, Christopher T.
 DEPARTMENT OF BIOLOGICAL CHEMISTRY AND MOLECULAR PHARMACOLOGY, HARVARD MEDICAL SCHOOL, BOSTON, MA, 02115, USA
 SOURCE: Journal of the American Chemical Society (1999), 121(17), 9716-9727
 CODEN: JACSAT; ISSN: 0002-7867
 PUBLISHER: American Chemical Society
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 AB: The presence of rigid structural elements such as thiazole and oxazole heterocyclic rings in peptide-derived compounds confers a wide range of therapeutic properties including antibacterial, antiviral, and antitumor activity. Using high resolution tandem mass spectrometry (MS/MS), we determine here the effect of heterocycle formation on MS/MS of reaction intermediates and use this unique MS/MS signature to ascertain the region- and chemoselectivity of microcin B7 synthetase.
 IT 8426-90-5, Microcin B7
 RI: B7O (Biological study, unclassified); NFM (Metabolic formation); B7O (Biological study); FOM (Formation, nonpreparative)
 NO 8426-90-5 CAPLUS
 CH 1-Isocysteine, L-valylglycyl-L-isoleucylglycylglycylglycylglycylglycylglycylglycyl-L-[2-(aminomethyl)-4-oxazolidinonylglycyl]-L-argyl-L-asparagylglycyl-L-[2-(aminomethyl)-4-thiazolidinonylglycyl]-L-argyl-L-asparagylglycyl-L-[2-(aminomethyl)-4-oxazolidinonylglycyl]-2-(aminomethyl)-4-oxazolidinonylglycyl-L-argyl-L-asparagylglycyl-L-[2-(aminomethyl)-4-thiazolidinonylglycyl]-L-argyl-L-asparagylglycyl-L-CA INDEX NAME
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 OC-CITING REF COUNT: 12 THERE ARE 12 CAPLUS RECORDS THAT CITE THIS RECORD (12 CITINRES)
 REFERENCE COUNT: 17 THERE ARE 17 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L31 ANMERK 33 OF 53 CAPLUS COPYRIGHT 2010 ACS ON STM
 ACCESSION NUMBER: 1999:563798 CAPLUS
 DOCUMENT NUMBER: 129:287745
 ORIGINAL REFERENCE NO.: 129:58587a,58578a
 TITLE: ATP/GTP hydrolysis is required for oxazole and thiazole biosynthesis in the peptide antibiotic microcin B7
 AUTHOR(S): Malm, Jill C.; Eliot, Andrew C.; Kelleher, Neil L.; Walsh, Christopher T.
 DEPARTMENT OF BIOLOGICAL CHEMISTRY, MOLECULAR PHARMACOLOGY HARVARD MEDICAL SCHOOL, BOSTON, MA, 02115, USA
 SOURCE: Biochemistry (1999), 37(18), 13252-13261
 CODEN: BICWAM; ISSN: 0006-2960
 PUBLISHER: American Chemical Society
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 AB: In the maturation of the *Escherichia coli* antibiotic microcin B7, the product of the mba gene is modified posttranslationally by the multistep microcin synthetase complex (composed of MbaA, C, and D) to cyclize four Cys and four Ser residues to four thiazoles and four oxazoles, resp. The purified synthetase shows an absolute requirement for ATP or GTP in peptide substrate heterocyclization, with GTP over-ethylid as effective as ATP in initial rate studies. The ATPase/GTPase activity of the synthetase complex is nonessential: it that ATP or GTP formation requires the presence of substrate noncylizable versions of MbaA bind to synthetase, but do not initiate the ATPase activity. The stoichiometry of ATP hydrolysis and heterocycle formation is 1:1 for a substrate that contains two potential sites of modification. However, at high substrate concn. (150mM) heterocycle formation is inhibited, while ATPase activity remains unaltered, consistent with uncoupling of ATP hydrolysis and heterocycle formation at high substrate concn. Sequence homol. reveals that the mbaC subunit has motifs reminiscent of the Walker B box in ATP utilizing enzymes and of motifs found in small G protein GTPases. Mutagenesis of three aspartates to alanine in these motifs (D212, D247, and D293) reduced microcin B7 production in vivo and heterocycle formation in vitro, suggesting that the 45 kDa MbaB has a regulated ATPase/GTPase domain in its N-terminal region necessary for peptide heterocyclization.
 IT 8426-90-5, Microcin B7
 RI: B7N (Biological study preparation); B7O (Biological study); PKP (Preparative)
 NO 8426-90-5 CAPLUS
 CH 1-Isocysteine, L-valylglycyl-L-isoleucylglycylglycylglycylglycylglycylglycyl-L-[2-(aminomethyl)-4-oxazolidinonylglycyl]-L-argyl-L-asparagylglycyl-L-[2-(aminomethyl)-4-thiazolidinonylglycyl]-L-argyl-L-asparagylglycyl-L-glutamylglycylglycyl-L-[2-(aminomethyl)-4-thiazolidinonylglycyl]-L-argyl-L-asparagylglycyl-L-[2-(aminomethyl)-4-oxazolidinonylglycyl]-2-(aminomethyl)-4-oxazolidinonylglycyl-L-argyl-L-asparagylglycyl-L-[2-(aminomethyl)-4-thiazolidinonylglycyl]-L-argyl-L-asparagylglycyl-L-CA INDEX NAME

L31 ANMERK 34 OF 53 CAPLUS COPYRIGHT 2010 ACS ON STM (Continued)
 *** STRUCTURE DIAGRAM IS NOT AVAILABLE ***
 OC-CITING REF COUNT: 38 THERE ARE 38 CAPLUS RECORDS THAT CITE THIS RECORD (18 CITINRES)
 REFERENCE COUNT: 41 THERE ARE 41 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L31 ANWER 34 OF 53 CAPLUS COPYRIGHT 2010 ACS ON STM (Continued)
 ACCESSION NUMBER: 1999;482687 CAPLUS
 DOCUMENT NUMBER: 129-20054
 ORIGINAL REFERENCE NO.: 129-470154
 TITLE: Thrombin receptor (PAR-1) antagonists.
 Abstract: Heterocycle-based peptidomimetics of the SPPLR agonist
 AUTHOR(S): Mokata, William J.; Hulschier, Becky L.; Mooney, David F.; Andrade-Oliveira, Patricia; Hoffmann, Jack
 A.I.
 ADD: Michael F.; Glusberg, Donna; Montemayor, Robert M.; Maydanoff, Bruce E.
 CORPATE SOURCE: The R. W. Scherer Pharmaceutical Research Institute, Spring House, PA, 15477, USA
 SOURCE: Bioorganic & Medicinal Chemistry Letters (1999), 9(13), 2449-2454
 COUNTRY: BRULUS; ISSN: 0960-894X
 PUBLICATION: Elsevier Science Ltd.
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 GI:

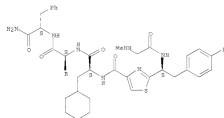


AB The thrombin receptor (PAR-1) is activated by α-thrombin to stimulate various cell types, including platelets, through the tetrapeptide-ligand sequence SPPLR. A series of oxazole- or thiazole-based oxazolidinones, designed after SPPLR, were synthesized and evaluated in vitro. The compounds inhibited platelet aggregation induced by SPPLR-MS or α-thrombin, and blocked the binding of [S]-Ser-(p-F)-Ser-Leu-Ser-(p-F)-Tyr-NO₂ (Ser = homoarginine) to a cAMP membrane preparation of PAR-1. Oxazole-based peptide 1 bound to PAR-1 with
 with
 IC₅₀ of 1.6 μM, and gave IC₅₀ values of 25 μM and 6.6 μM against α-thrombin- and SPPLR-MS-induced platelet aggregation, resp.
 IT
 212756-41-7P 212756-47-3P 212756-48-4P
 212756-49-5P 212756-50-6P 212756-52-1P
 212756-54-2P 212756-55-3P 212756-56-4P
 212756-57-5P 212756-58-6P 212756-59-7P
 212756-60-2P 212756-61-1P 212756-62-2P
 EL: RAC (biological activity or effector, except adverse); RDU
 (biological
 study, unclassified); SPH (Synthetic preparation); RGL (Biological study); PRP (Preparation)
 (preparation of oxazole- and thiazole-based peptidomimetics as thrombin receptor antagonists)
 NI 212756-41-7 CAPLUS

L31 ANWER 34 OF 53 CAPLUS COPYRIGHT 2010 ACS ON STM (Continued)
 CS 1-Phenylalaninamide, N-methylglycyl-2-[(1S)-3-amino-2-(4-fluorophenylethyl)-4-thiazolecarboxyl-3-cyclohexyl-5-allyl-L-arginyl]- (PCI) (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A



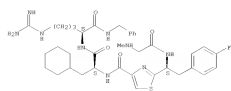
PAGE 2-A



NI 212756-49-5 CAPLUS
 CS 1-Phenylalaninamide, L-valyl-2-[(1S)-3-amino-2-(4-fluorophenylethyl)-4-thiazolecarboxyl-3-cyclohexyl-5-allyl-L-arginyl]- (PCI) (CA INDEX NAME)

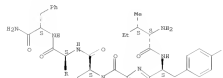
Absolute stereochemistry.

L31 ANWER 34 OF 53 CAPLUS COPYRIGHT 2010 ACS ON STM (Continued)
 CS 1-Arginylamide, N-methylglycyl-2-[(1S)-3-amino-2-(4-fluorophenylethyl)-4-thiazolecarboxyl-3-cyclohexyl-5-allyl-L-phenylmethyl]- (PCI) (CA INDEX NAME)
 Absolute stereochemistry.



NI 212756-47-3 CAPLUS
 CS 1-Phenylalaninamide, L-isoleucyl-2-[(1S)-3-amino-2-(4-fluorophenylethyl)-4-thiazolecarboxyl-3-cyclohexyl-5-allyl-L-arginyl]- (PCI) (CA INDEX NAME)
 Absolute stereochemistry.

PAGE 2-A



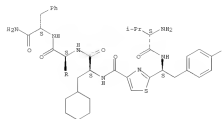
PAGE 2-A



NI 212756-68-4 CAPLUS

L31 ANWER 34 OF 53 CAPLUS COPYRIGHT 2010 ACS ON STM (Continued)

PAGE 1-A



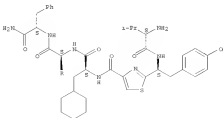
PAGE 2-A



NI 212756-50-8 CAPLUS
 CS 1-Phenylalaninamide, L-valyl-2-[(1S)-3-amino-2-(4-methoxyphenylethyl)-4-thiazolecarboxyl-3-cyclohexyl-5-allyl-L-arginyl]- (PCI) (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A

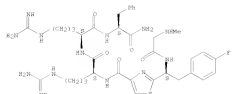


PAGE 2-A



HN 212756-53-1 CAPLUS
CN L-Phenylalaninamide, N-methylglycyl-2-[(1S)-3-amino-2-(4-fluorophenyl)ethyl]-4-thiazolecarboxyl-L-arginyl-L-arginyl- (PCI) (CA INDEX NAME)

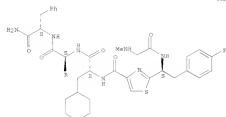
Absolute stereochemistry.



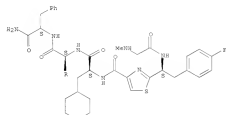
HN 212756-54-2 CAPLUS
CN L-Phenylalaninamide, N-methylglycyl-2-[(1R)-3-amino-2-(4-fluorophenyl)ethyl]-4-thiazolecarboxyl-3-cyclohexyl-D-alanyl-L-arginyl- (PCI) (CA INDEX NAME)

Absolute stereochemistry.

PAGE 3-A



PAGE 1-A

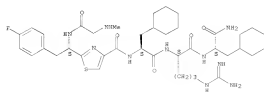


PAGE 2-A



HN 212756-57-3 CAPLUS
CN L-Alaninamide, N-methylglycyl-2-[(1R)-3-amino-2-(4-fluorophenyl)ethyl]-4-thiazolecarboxyl-3-cyclohexyl-L-alanyl-L-arginyl-3-cyclohexyl- (PCI) (CA INDEX NAME)

Absolute stereochemistry.



HN 212756-58-6 CAPLUS
CN Benzenesulfonamide, N-methylglycyl-2-[(1S)-3-amino-2-(4-fluorophenyl)ethyl]-4-thiazolecarboxyl-3-cyclohexyl-L-alanyl-L-arginyl-D-amino-, (aB)- (PCI) (CA INDEX NAME)

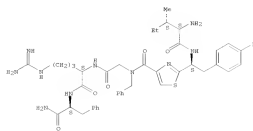
Absolute stereochemistry.

PAGE 2-A



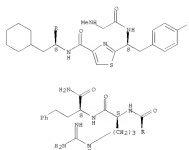
HN 212756-55-3 CAPLUS
CN L-Phenylalaninamide, L-isoleucyl-2-[(1S)-3-amino-2-(4-fluorophenyl)ethyl]-4-thiazolecarboxyl-L-phenylmethylglycyl-L-arginyl- (PCI) (CA INDEX NAME)

Absolute stereochemistry.



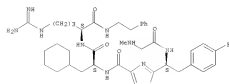
HN 212756-56-4 CAPLUS
CN L-Phenylalaninamide, N-methylglycyl-2-[(1S)-3-amino-2-(4-fluorophenyl)ethyl]-4-thiazolecarboxyl-3-cyclohexyl-L-alanyl-3H-aminoinosinyl-L-lysyl- (PCI) (CA INDEX NAME)

Absolute stereochemistry.



HN 212756-59-7 CAPLUS
CN L-Arginanimide, N-methylglycyl-2-[(1R)-3-amino-2-(4-fluorophenyl)ethyl]-4-thiazolecarboxyl-3-cyclohexyl-L-alanyl-N-(2-phenylethyl)- (PCI) (CA INDEX NAME)

Absolute stereochemistry.



HN 212756-60-6 CAPLUS
CN L-Arginanimide, N-methylglycyl-2-[(1R)-3-amino-2-(4-fluorophenyl)ethyl]-4-thiazolecarboxyl-L-lysyl-N-(2-phenylethyl)- (PCI) (CA INDEX NAME)

Absolute stereochemistry.

L31 ANSWER 39 OF 53 CAPLUS COPYRIGHT 2010 ACS on STN (Continued)
 08-CITING REF COUNT: 42 THERE ARE 42 CAPLUS RECORDS THAT CITE THIS
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ACCESSION NUMBER: 013 ANIMEN 405 OF 53
 ACCESSION NUMBER: 013 ANIMEN 405 OF 53
 DOCUMENT NUMBER: 013 ANIMEN 405 OF 53
 ORIGINAL REFERENCE NO.: 013 ANIMEN 405 OF 53
 TITLE: 013 ANIMEN 405 OF 53
 define 013 ANIMEN 405 OF 53
 AUTHOR(S): 013 ANIMEN 405 OF 53
 COOPERATIVE SOURCE: 013 ANIMEN 405 OF 53
 G2115, 013 ANIMEN 405 OF 53
 SOURCE: 013 ANIMEN 405 OF 53
 COUNTRY: 013 ANIMEN 405 OF 53
 DOCUMENT TYPE: 013 ANIMEN 405 OF 53
 LANGUAGE: 013 ANIMEN 405 OF 53
 ABSTRACT: 013 ANIMEN 405 OF 53
 into 013 ANIMEN 405 OF 53
 two structural classes, the quinolones and the coumarins. A third class
 of RNA gyrase inhibitor is defined by the rationally synthesized peptide
 residues. 013 ANIMEN 405 OF 53
 of these are posttranslationally modified. Here the authors
 describe the characterization of the structure of these modifications.
 The authors propose that four cysteine and four serine side chains
 undergo
 condensation with the carbonyl group of the preceding serine, followed
 by
 a/polycondensation to yield four thiazole and four
 thiazolidine rings. The authors propose that the catalyzing these
 modifications (HMBSD) would constitute the only thiazole
 nucleoside biosynthesis. The authors propose that the authors open up
 possibilities for the design of RNA gyrase inhibitors and to the
 general class of posttranslational modifications with potential protein
 engineering. Kechrischiella sibi sibi mutants, which lack the inner
 protein (ISB) involved in HMBSD uptake, were found to be resistant to
 thiazole. Nucleoside is structurally unique. HMBSD except for the
 fact that it contains a thiazole ring. This suggests that the
 thiazole rings are part of the HMBSD structure recognized by
 the enzyme. This observation is consistent with the fact that the widely
 conserved and can play developmental roles (Glasgow, S. J., Ziegler, A. S.
 and S. J. Ziegler, 1978). The authors propose that the thiazole and
 thiazole and coumarin-containing compounds may serve as signaling molecules
 in a wide variety of biological processes. The authors propose that the

L31 ANMER 40 OF 53 CAPLUS COPYRIGHT 2010 ACS ON STN (Continued)

(aminomethyl)-4-thiazolocarboxyl-L-acyl-L-asparagyl-2-[2-(aminomethyl)-4-thiazolyl]-4-oxalocarboxylglycylglycyl-L-asparagylglycyl-2-(aminomethyl)-4-oxalocarboxylglycyl-2-(aminomethyl)-4-oxalocarboxylglycyl-L-acyl-L-histidyl- (CA INDEX NAME)

*** STRUCTURE DIAGRAM IS NOT AVAILABLE ***

OS-CITING REF COUNT: 62 THERE ARE 62 CAPLUS RECORDS THAT CITE THIS RECORD (62 CITINGS)

L31 ANMER 41 OF 53 CAPLUS COPYRIGHT 2010 ACS ON STN (Continued)

ACCESSION NUMBER: 1993:419496 CAPLUS

DOCUMENT NUMBER: 119:419496

ORIGINAL REFERENCE NO.: 119:390126, 390134

TITLE: Post-translational backbone modification via heterocyclic five-membered ring formation during the biosynthesis of the glycine-rich antibiotic microcin B17

AUTHOR(S): Bayer, Anja Freund; Stefany Nicholson; Gerny Jung; Guehler Inst.-Org. Chem., Univ. Tübingen, Tübingen, D-72076, Germany

SOURCE: Angewandte Chemie (1993), 105(9), 1410-13 (See also Angew. Chem., Int. Ed. Engl., 1993, 32(9), 1331-9) CROSS REF: JCRN: 9044-1543

DOCUMENT TYPE: Journal General Review

LANGUAGE: German

AB A review, with 14 refs., on the posttranslational modification of a peptide antibiotic, microcin B17, in which serine and cysteine residues undergo cyclization into 5-membered heterocyclic oxazoline and thiazoline rings.

IT 84286-90-5, Microcin B17

EL: PROC (Process)

Posttranslational modification of)

IN 84286-90-8 CAPLUS

CH L-Isoleucine, L-valylglycyl-L-

isoleucylglycylglycylglycylglycylglycylglycylglycylglycylglycyl-L-[2-(aminomethyl)-4-oxalonyl]-4-thiazolocarboxylglycyl-L-glutamylglycylglycyl-L-(aminomethyl)-4-thiazolocarboxylglycyl-2-

(aminomethyl)-4-thiazolocarboxyl-L-acyl-L-asparagyl-2-[2-(aminomethyl)-4-thiazolyl]-4-oxalocarboxylglycylglycyl-L-asparagylglycyl-2-(aminomethyl)-4-oxalocarboxylglycyl-3-(aminomethyl)-4-oxalocarboxylglycyl-L-acyl-L-histidyl- (CA INDEX NAME)

*** STRUCTURE DIAGRAM IS NOT AVAILABLE ***

OS-CITING REF COUNT: 3 THERE ARE 3 CAPLUS RECORDS THAT CITE THIS RECORD (3 CITINGS)

L31 ANMER 42 OF 53 CAPLUS COPYRIGHT 2010 ACS ON STN

ACCESSION NUMBER: 1993:475964 CAPLUS

DOCUMENT NUMBER: 119:475964

ORIGINAL REFERENCE NO.: 119:131976, 131984

TITLE: Synthesis of the isomer of cyclopeptide acetylacyclamide

AUTHOR(S): Jian, Zhigang; Jian, Dunlong; Long, Wanhong; Dep. Chem., Zhongshan Univ., Canton, 510275, Peop. Rep. China

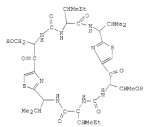
SOURCE: Zhongshan Daxue Xuebao, Sine Xuewen (1992), 31(2), 57-61

CODEN: CHTXAJ; ISSN: 0529-6579

DOCUMENT TYPE: Journal

LANGUAGE: Chinese

62



I

AB The title compound (I) has been synthesized. The thiazole amino acid was prepared by Rastbach method. The peptide bonds were

constructed by

DCC-DMAP (DCC = dicyclohexylcarbodiimide, DMAP = 4-dimethylaminopyridine) coupling method and the peptide ring was formed by azide method.

IT 149186-61-9 149186-61-9

EL: PROC (Process)

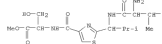
Preparation and cyclization of)

IN 149186-61-9 CAPLUS

CH L-Isoleucine, L-isoleucyl-2-[1-(amino-2-methylpropyl)-4-thiazolocarboxyl-1-

methylester, 4-hydroxybutanoate (HCBT) (CA INDEX NAME)

L31 ANMER 42 OF 53 CAPLUS COPYRIGHT 2010 ACS ON STN (Continued)

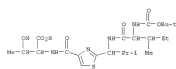


●: NCL

IN 149186-61-9 CAPLUS

CH L-Threonine,

N-[[2-[1-[2-[[1-[1-[1,1-dimethylethoxy]carbonyl]amino]-3-methyl-1-oxopropyl]amino]-2-methylpropyl]-4-thiazolyl]carbonyl]- (9CI) (CA INDEX NAME)



IT 175608-17-9P

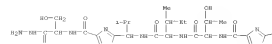
EL: RCT (Reactant); RHM (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

Preparation and cyclization of)

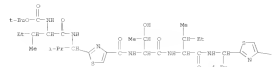
IN 175608-13-8 CAPLUS

CH L-Isoleucine, N-[[2-[1-[1-[2-(amino-3-methyl-1-oxopropyl]amino]-2-methylpropyl]-4-thiazolyl]carbonyl]-L-thiazolyl]-L-thiazolyl-2-[[2-hydroxy-1-(hydroxymethyl)-2-oxopropyl]amino]carbonyl]-2-thiazolyl]-2-methylpropyl- (9CI) (CA INDEX NAME)

PAGE 3-A



IT 135401-12-7P
 Re: KCT (Reactant) SYN (Synthetic preparation); PREP (Preparation); NACT (Reactant or reagent)
 [preparation and deprotection of]
 RE 135405-12-7 CAPLUS
 CH 1-isoleucineamide, N-[[2-[1-[[[1,1-dimethylethoxy]carbonyl]amino]-3-methyl-1-oxopropyl]amino]-2-methylpropyl]-4-thiazolyl]methyl]-1-threonyl-N-[[4-[[1-[(2-hydroxyethyl)-2-methoxy-2-oxoethyl]amino]acetyl]-2-thiazolyl]-2-methylpropyl]- (9C1) (CA INDEX NAME)

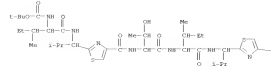
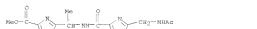


IT 135408-11-6P
 Re: KCT (Reactant) SYN (Synthetic preparation); PREP (Preparation); NACT (Reactant or reagent)
 [preparation and deprotection of]
 RE 135405-11-6 CAPLUS
 CH 1-isoleucineamide, N-[[2-[1-[[[1,1-dimethylethoxy]carbonyl]amino]-3-methyl-1-oxopropyl]amino]-2-methylpropyl]-4-thiazolyl]methyl]-1-threonyl-N-[[4-[[1-[(2-hydroxyethyl)-2-methoxy-2-oxoethyl]amino]acetyl]-2-thiazolyl]-2-methylpropyl]- (9C1) (CA INDEX NAME)

L31 ANMERK 43 OF 53 CAPLUS COPYRIGHT 2010 ACS ON STM
 ACCESSION NUMBER: 1393;546817 CAPLUS
 DOCUMENT NUMBER: 117;110250
 ORIGINAL REFERENCE NO.: 117;135794;19582a
 TITLE:
 The structures of A10225 B, -G and -I: new thapsigargin antibiotics produced by Streptomyces gardenii
 AUTHOR(S):
 Debono, Manuel; Muller, P. Michael; Concolviti, John L.; Paschal, Jonathan W.; Hunt, Ann B.; Michel, Karl E.; Martin, James W.
 COMPANY SOURCE:
 Lilly Corp., Dept., Indianapolis, IN, 46285, USA
 SOURCE:
 Journal of Organic Chemistry (1992), 57(19), 5200-8
 CODEN: JOCHAY, ISSN: 0022-3263
 DOCUMENT TYPE:
 Journal
 LANGUAGE:
 English
 AB: The structures of the major members of a new family of important thapsigargin antibiotics, A10225 (I), A10250 (II), and A10252 (III), provided by S. gardenii (NO. 15537) are described. Selective chemical degradation in combination with IR, FAB/MS, and CID methods on the degradation products was required to solve these structures. Methanolysis of I resulted in the isolation of 4-methoxy-2-propionylisoleucine and di-methylsilylacetate as well as N-(acetamidomethyl)thiazolyl]-1-(acetamidomethyl)thiazolyl]ethanamide after acetylation. Vigorous treatment with acid produced benzoylamine acid. Trifluoroacetic acid led to cleavage at the 6 and 7 positions residues to give a complex and highly modified pentapeptide which was sequenced by CID/MS and IR techniques. The pentapeptide was composed of alliphosphonate acid, threonine, 1-(4-carboxyphenyl)-1-aminopropyl amine (dehydroisovaline masked by aspartate at its carboxyl group), 2-aminomethylthiazole 4-carboxylic acid, and 2-(1-aminomethyl)-4-carboxybenzothiazole. FAB/MS

base hydrolysis showed that I had a dehydroisovaline tetrapeptide side chain. Antithion II and III each had a masked dehydrobutyran in place of the dehydroisovaline present in I, and III had a single masked dehydroisovaline as a side chain.
 IT 14154-29-4P
 Re: SYN (Synthetic preparation); PREP (Preparation)
 [preparation of]
 RE 141746-31-3 CAPLUS
 CH 4-thiazolecarboxylic acid, 2-[1-[[[2-(acetylaminomethyl)-4-thiazolyl]methyl]amino]methyl]-, methyl ester (CA INDEX NAME)

OR-CITING REF COUNT: 17 THERE ARE 17 CAPLUS RECORDS THAT CITE THIS RECORD (17 CITINGS)

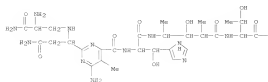


L31 ANMERK 44 OF 53 CAPLUS COPYRIGHT 2010 ACS ON STM
 ACCESSION NUMBER: 1393;510250 CAPLUS
 DOCUMENT NUMBER: 117;110250
 ORIGINAL REFERENCE NO.: 117;135794;19582a
 TITLE:
 On the role of individual thiazole moieties in oxygen activation and DNA cleavage
 AUTHOR(S):
 Hummel, Horst; Natter, Hans; Licht, Sidney M.
 COMPANY SOURCE:
 Karl. Desh. Univ. Virginia, Charlottesville, VA, 22901, USA
 SOURCE:
 Journal of the American Chemical Society (1992), 114(18), 6788-91
 CODEN: JACSAT, ISSN: 0002-7863
 DOCUMENT TYPE:
 English
 OTHER SOURCE(S):
 CASREACT 117-110250

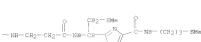
* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

AB: Two structurally novel thiazole (TH) analogs I and II were prepared by total synthesis to permit the evaluation of the role of individual thiazole moieties in the processes of thiazole-mediated oxygen activation and DNA degradation. Each of the compounds was structurally related to dephosphorylated dimethyl A1 but contained an N-methyl-L-cysteine moiety in lieu of one of the two thiazoles normally present in thiazole. In common with thiazole and dephosphorylated, both monothiazole THs were found to be excellent catalysts for the oxygenation of low mol. weight substrates such as naphthalene and styrene and also mediated the demethylation of N,N-dimethylamine. However, both of the monothiazole THs were much less effective than thiazole or dephosphorylated in promoting DNA degradation. Anal. of the effects of the monothiazole THs on 5'- and 3'-3'P and labeled DNA duplexes indicated that cleavage occurred without discernible sequence specificity. These results demonstrate that the thiazole moiety as RUP is not required for O2 activation or for the oxygenation and oxidation of low mol. substrates as what are presumably bimol. processes. However, the thiazole clearly does contribute to the efficiency of thiazole-mediated DNA degradation and to the sequence selectivity of DNA strand scission by thiazole.
 IT 141721-45-7
 Re: KCT (Reactant); NACT (Reactant or reagent)
 [oxygen activation and DNA cleavage by]
 RE 141721-45-7 CAPLUS
 CH 1-thiazolecarboxylic acid, 4-[2-O-de[2-O-[3-O-(aminocarbonyl)-5-m-methoxypropyl]-5-m-gulopropyl]-8,10-dimethyl-7,9,10,11-tetrahydro-8-methylthio]-N-[1-(methylthio)propyl]-10-oxo-, (7S)- (9C1) (CA INDEX NAME)

PAGE 1-A

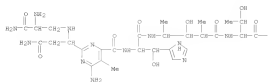


PAGE 1-B

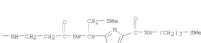


22 142721-65-7 CAPLUS
 CN β -Alaninamide, 4-[3-O-*tert*-butyl (aminoacetyl)- α -D-mannopyranosyl]- α -L-glucopyranosyl]-9,10-deepithio-7,8,10,11-tetrahydro-8-methylthio-N-[1,4-[[[3-(methylthio)propyl]amino]carboxyl]-2-thiazolyl]ethyl]-, (7S)- (PCT) (CA INDEX NAME)

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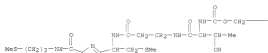


PAGE 1-B



22 142721-63-9 CAPLUS
 CN β -Alaninamide, N-[1,2,2-trisubstituted (ethoxycarbonyl)-L-threonyl-N-[2-(methylthio)-1,4-[[[3-(methylthio)propyl]amino]carboxyl]-2-thiazolyl]ethyl]-, (S)- (PCT) (CA INDEX NAME)

PAGE 1-A

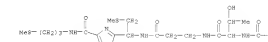


PAGE 1-B

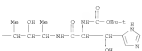


22 142721-65-1 CAPLUS
 CN β -Alaninamide, 2,4,5-trideoxy-4-[[[2-[[[1,1-dimethylthio]ethyl]amino]carboxyl]-2-hydroxy-1-[18-imidazol-4-yl]-1-oxopropyl]amino]-N-[2-hydroxy-1-[[[3-(methylthio)propyl]amino]carboxyl]-2-thiazolyl]ethyl]amino]-2-oxopropyl]amino]carboxyl]propyl]-2-methyl-, [1,18(S), 2(S), 4(2S,3S)]- (PCT) (CA INDEX NAME)

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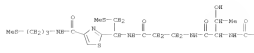
PAGE 1-B



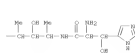
22 142721-67-3 CAPLUS

IT 142721-66-2P
 RL PCT (Reactant); SRN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
 [Preparation and coupling of, with pyrimidinobisamide acid]
 CN 142721-66-2 CAPLUS
 CN β -Alaninamide, 4-[[[2-amino-3-hydroxy-3-(18-imidazol-4-yl)-1-oxopropyl]amino]-2,4,5-trideoxy-N-[2-hydroxy-1-[[[2-[[[methylthio]-1-[[[3-(methylthio)propyl]amino]carboxyl]-2-thiazolyl]ethyl]amino]-3-oxopropyl]amino]carboxyl]propyl]-2-methyl-, [1,18(S), 2(S), 4(2S,3S)]- (PCT) (CA INDEX NAME)

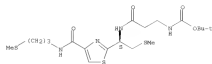
PAGE 1-A



PAGE 1-B

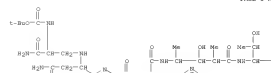


IT 142721-60-6P 142721-63-9D 142721-65-1P
 142721-67-3D
 RL PCT (Reactant); SRN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
 [Preparation and deblocking of]
 CN 142721-60-6 CAPLUS
 CN Carboxylic acid, [3-[[[2-(methylthio)-1,4-[[[3-(methylthio)propyl]amino]carboxyl]-2-thiazolyl]ethyl]amino]-3-oxopropyl]-1,1-dimethyl ethyl ester, (S)- (PCT) (CA INDEX NAME)
 Absolute stereochemistry.



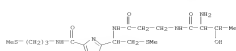
L31 ANSWER 44 OF 53 CAPLUS COPYRIGHT 2010 ACS on STN (Continued)
 CN β -Alaninamide, 4-[3-O-*tert*-butyl (aminoacetyl)- α -D-mannopyranosyl]- α -L-glucopyranosyl]-8,10-deepithio-838-[[1,1-dimethylethoxy]carboxyl]-7,8,10,11-tetrahydro-8-methylthio-N-[1-(methylthio)propyl]-10-oxo-, (7S)- (PCT) (CA INDEX NAME)

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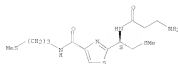


PAGE 1-B

IT 142721-64-0P
 RL PCT (Reactant); SRN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
 [Preparation and peptide coupling of, with dipeptide derivative]
 CN 142721-64-0 CAPLUS
 CN β -Alaninamide, L-threonyl-N-[2-(methylthio)-1,4-[[[3-(methylthio)propyl]amino]carboxyl]-2-thiazolyl]ethyl]-, (S)- (PCT) (CA INDEX NAME)

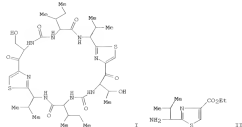


L31 ANWER 44 OF 53 CAPLUS COPYRIGHT 2010 ACS ON STM (Continued)
 IT 141721-61-7P
 RI: RCT (Reactant); SPM (Synthetic preparation); PREP (Preparation); RACT
 (Reactant or reagent)
 RI 141721-61-7 CAPLUS
 CH 4-thiazolaceticamide, 2-[[1-[(3-amino-1-oxopropyl)amino]-2-
 methylthioethyl]-6-[3-(methylthio)propyl]-, (S)- (PCI) (CA INDEX NAME)
 Absolute stereochemistry.



OS: CITING REF OXBT: 25 THERE ARE 25 CAPLUS RECORDS THAT CITE THIS
 RECORD (27 CITINGS)

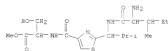
L31 ANWER 45 OF 53 CAPLUS COPYRIGHT 2010 ACS ON STM (Continued)
 ACCESSION NUMBER: 1991:515071 CAPLUS
 DOCUMENT NUMBER: 115115571
 ORIGINAL REFERENCE NO.: 11519754, 19754
 TITLE: Synthesis of cyclopeptide EL-(Val)Tha-4-Sar-1-11a
 L-11a-L-Thr-Ole-(Val)Tha
 AUTHOR (S): Jian, Zhiqiang; Jian, Dunlong; Long, Kangshou
 Dep. Chem., Zhongshan Univ., Canton, P. Rep. China
 SOURCE: Zhongguo Huaxue Jikan (1990), 9(17), 1-4
 CORDIS CATEGORY: JSM: 1990-1461
 DOCUMENT TYPE: Journal
 LANGUAGE: Chinese
 CI



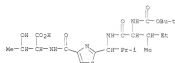
AB The title cyclopeptide (I) was prepared from L-serine, L-threonine,
 L-isoleucine, and thiazole II. Peptide ring was formed by azide
 method.

IT 135607-97-5P 135607-99-7P 135602-32-5P
 135602-34-7P
 RI: RCT (Reactant); SPM (Synthetic preparation); PREP (Preparation); RACT
 (Reactant or reagent)
 (Preparation and coupling reaction of)
 RI 135607-97-5 CAPLUS
 CH L-Serine,
 L-isoleucyl-2-[[15]-1-amino-2-methylpropyl]-4-thiazolacarbonyl-,
 methyl ester, dihydrochloride (PCI) (CA INDEX NAME)

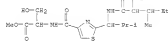
L31 ANWER 46 OF 53 CAPLUS COPYRIGHT 2010 ACS ON STM (Continued)



RI 135601-99-7 CAPLUS
 CH L-Threonine,
 N-[[2-[[1-[[1,3-dimethylethoxy]carbonyl]amino]-3-methyl-1-
 oxopropyl]amino]-2-methylpropyl]-4-thiazolyl]carbonyl]-,
 [2S-[1R*,2R*,3R*]]- (PCI) (CA INDEX NAME)

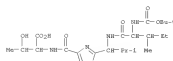


RI 135602-32-5 CAPLUS
 CH L-Serine,
 L-isoleucyl-2-[[18]-1-amino-2-methylpropyl]-4-thiazolacarbonyl-,
 methyl ester, dihydrochloride (PCI) (CA INDEX NAME)



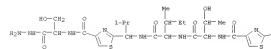
RI 135602-34-7 CAPLUS
 CH L-Threonine,
 N-[[2-[[1-[[1,3-dimethylethoxy]carbonyl]amino]-3-methyl-1-
 oxopropyl]amino]-2-methylpropyl]-4-thiazolyl]carbonyl]-,
 [2S-[1R*,2R*,3R*]]- (PCI) (CA INDEX NAME)

L31 ANWER 47 OF 53 CAPLUS COPYRIGHT 2010 ACS ON STM (Continued)



IT 135608-12-8P
 RI: RCT (Reactant); SPM (Synthetic preparation); PREP (Preparation); RACT
 (Reactant or reagent)
 (Preparation and cyclization of)
 RI 135608-13-8 CAPLUS
 CH N-[[2-[[1-[[10-amino-3-methyl-1-oxopropyl]amino]-2-
 methylpropyl]-4-thiazolyl]carbonyl]-L-threonyl-N-[[1-4-[[12-hydroxy-1-
 (hydroxyethyl)-2-oxethyl]amino]carbonyl]-2-thiazolyl]-2-methylpropyl]-
 (PCI) (CA INDEX NAME)

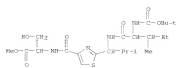
PAGE 1-A



PAGE 1-B

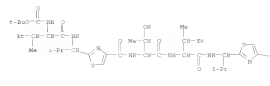


IT 135607-96-4P 135608-12-7P 135602-31-4P
 RI: RCT (Reactant); SPM (Synthetic preparation); PREP (Preparation), RACT
 (Reactant or reagent)
 (Preparation and deprotection of)
 RI 135607-96-4 CAPLUS
 CH L-Serine, N-[[2-[[1-[[1,3-dimethylethoxy]carbonyl]amino]-3-methyl-1-
 oxopropyl]amino]-2-methylpropyl]-4-thiazolyl]carbonyl]-, methyl ester,
 [2S-[1R*,2R*,3R*]]- (PCI) (CA INDEX NAME)



RU 135408-11-7 CAPLUS
 CH 1-isoxazolinane, N-[2-[[1-[[[1,3-dimethylethoxy]carbonyl]amino]-3-methyl-1-isoxazolinane]-2-methylpropyl]-4-thiazolyl]carbamoyl]-L-threonine-1-Ph
 N-[3-[[1-[[[1,3-dimethylethoxy]carbonyl]amino]-2-methylpropyl]-4-thiazolyl]-2-methylpropyl]-1-Ph (PC) (CA INDEX NAME)

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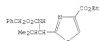


PAGE 1-B



RU 135408-11-4 CAPLUS
 CH 1-isoxazolinane, N-[2-[[1-[[[1,3-dimethylethoxy]carbonyl]amino]-3-methyl-1-isoxazolinane]-2-methylpropyl]-4-thiazolyl]carbamoyl]-, methyl ester, [2S-[2(2*),2R*,2R*]]- (PC) (CA INDEX NAME)

L31 ANSWER 46 OF 53 CAPLUS COPYRIGHT 2010 ACS on STN
 ACCESSION NUMBER: 135408-11-4 CAPLUS
 DOCUMENT NUMBER: 113115828
 ORIGINAL REFERENCE NO.: 113115828, 1965-4a
 TITLE: Synthesis of heptapeptide
 1le-Thr-(Val)Thr-1le-Thr-(Val)Thr
 Jian, Dunlong Long, Kangshu
 Chen, Dep., Zhongshan Univ., Canton, Peop. Rep. China
 SOURCE: Yinyong Huaxue (1969), 6(5), 77-80
 CDB: 178780; 2880; 1000-0558
 Jernall
 CHINESE
 DOCUMENT TYPE: CHEMICAL
 OTHER SOURCE(S): CASREACT 113115828
 GI

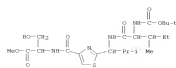
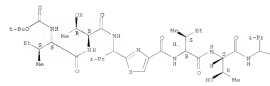


AB Heptapeptide 1le-Thr-(Val)Thr-1le-Thr-(Val)Thr, the ring opening product of
 acylurethane, was synthesized. The (Val)Thiazole amino acid
 derivative 1 was prepared by Hantzsch method.

IT 12855-43-49
 RU 12855-43-49
 CH 1-isoxazolinane, N-[2-[[1-[[[1,3-dimethylethoxy]carbonyl]amino]-3-methyl-1-isoxazolinane]-2-methylpropyl]-4-thiazolyl]carbamoyl]-L-threonine-1-Ph
 N-[3-[[1-[[[1,3-dimethylethoxy]carbonyl]amino]-2-methylpropyl]-4-thiazolyl]-2-methylpropyl]-1-Ph (PC) (CA INDEX NAME)

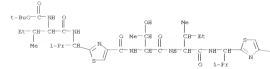
Absolute stereochemistry.

PAGE 1-A



IT 135408-11-49
 RU 135408-11-49
 CH 1-isoxazolinane, N-[2-[[1-[[[1,3-dimethylethoxy]carbonyl]amino]-3-methyl-1-isoxazolinane]-2-methylpropyl]-4-thiazolyl]carbamoyl]-L-threonine-1-Ph
 N-[3-[[1-[[[1,3-dimethylethoxy]carbonyl]amino]-2-methylpropyl]-4-thiazolyl]-2-methylpropyl]-1-Ph (PC) (CA INDEX NAME)

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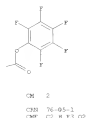


PAGE 1-B

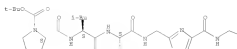


PAGE 1-B

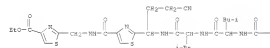




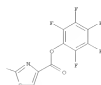
IT 111285-49-SP
 R1a RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
 (Reactant or reagent)
 (preparation and delocking of)
 NH 111282-48-8 CAPLOS
 CH 1-Valineamide, 1-[[[1,1-dimethylethoxy]carbonyl]-L-prolyl-L-leucyl]-N-[[4-
 [[[(4-[[[pentafluorophenyl]carbonyl]-2-thiazolyl]methyl]amino]carbonyl]-2-
 thiazolyl]methyl]- (R)- (C4 INDEX NAME)
 Absolute stereochemistry.



L31 ANSWER 49 OF 53 CAPLOS COPYRIGHT 2010 ACS ON STN
 ACCESSION NUMBER: 138838343 CAPLOS
 DOCUMENT NUMBER: 10838343
 ORIGINAL REFERENCE NO.: 1084635a,443a
 TITLE: Amino acids and peptides. 60. Synthesis of biologically active cyclopeptides. 10. Synthesis of 16 structural isomers of dolastatin 3. II.
 Synthesis of the linear educts and the cyclopeptides
 AUTHOR(S): Schmidt, Ulrich; Ols, Roland; Lieberknecht, Albrecht;
 Gressner, Helmut; Potzoll, Bernd; Kahr, Johann;
 Wagner, Karin; Fischer, Peter
 CORPORATE SOURCE: Institut für Organische Chemie, Universität Stuttgart,
 D-70550, Fed. Rep. Ger.
 SOURCE: Synthesis (1997), (7), 216-41
 CODE(S): SYNREP; ISSN: 0039-1881
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 OTHER SOURCE(S): CASREACT 10838343
 QT For diagrams, see printed CA issue.
 AS Sixteen isomers (I and II) of the macrocyclic cyclopeptide dolastatin 3 were synthesized. The proposed structure of dolastatin 3 is shown by 18 100% spectrometry to be incorrect.
 IT 8211-92-1P
 R1a RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
 (Reactant or reagent)
 (preparation and delocking-cyclization of)
 NH 9211192-1 CAPLOS
 CH 2-Valineamide, 1-[[[1,1-dimethylethoxy]carbonyl]-D-prolyl-D-leucyl]-N-[3-
 cyano-1-(4-[[[4-(ethoxycarbonyl)-2-thiazolyl]methyl]amino]carbonyl]-2-
 thiazolyl]propyl]-, (R)- (R)- (R)- (C4 INDEX NAME)



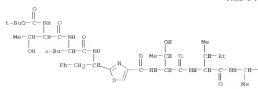
CS-CITING REF COUNT: 16 THERE ARE 16 CAPLOS RECORDS THAT CITE THIS RECORD (16 CITINGS)



CS-CITING REF COUNT: 4 THERE ARE 4 CAPLOS RECORDS THAT CITE THIS RECORD (4 CITINGS)

131 ANSWER 50 OF 53 CAPLUS COPYRIGHT 2010 ACS on STM (Continued)
(SCI) (CA INDEX NAME)

PAGE 1-3



PAGE 1-B

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

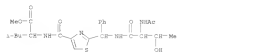
As the structures of patellanides A, B, and C have been proposed to be cyclic peptides I, II, and III, resp. I and II were synthesized by solution methods, but these synthetic peptides were not identical with natural patellanides B and C. An inspection of evidences used for the originally assigned structures and a synthetic study on the partial hydrolyzate of patellanide B indicated that the structures of patellanides B and C could be reassigned as cyclic peptides IV and V, resp., having the reverse

of amino acid residues. This deduction was confirmed by the syntheses of revised structures IV and V, which were completely identical with natural patellanides B and C, resp. The structures of patellanide A was analogously revised as cyclic peptide VI by its synthesis.

2T 106392-

KL: P3P (Properties)

CN 1-Laucine, N-[[[2-[[[2-(acetylamino)-3-hydroxy-1-oxobutyl]amino]phenyl]ethyl]-4-thiazolyl]carbonyl]-, methyl ester, [2S-[1(S*),2R*,3S*]]- (3CI) (CA INDEX NAME)



3F 101924-76-9P 101924-86-9P 102409-00-7P

103929-29-9P

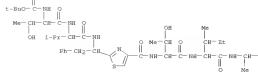
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and deblocking-cyclization of)

CN L-Isoleucinamide, N-[2-[1-[N-[N-[1,1-dimethylethoxy)carbonyl]-L-alloethreonyl]-L-leucyl]amino]-2-phenylethyl]-4-thiazolylcarbonyl]-L-alloethreonyl-N-[1-[4-(methoxycarbonyl)-2-thiazolyl]ethyl]-, [R-(R*,R*)]-

101924-84-2 CATALYTIC

L-Isolucaninamide, N-[1-[2-[1-[[N-[R-[[1,1-dimethylethoxy)carbonyl]-L-allo-threonyl]-L-valyl]amino]-2-phenylethyl]-4-thiazolyl]carbonyl]-L-allo-threonyl-N-[1-[4-[[ethoxycarbonyl]-2-thiazolyl]ethyl]-, [R-(R*,R*)]-(SC1) (CA INDEX NAME)

PAGE 1-A



1.31 ANSWER 50 OF 53 CASHIER COPYRIGHT 2010 ACS on BTN (Cont 5 more)

PAGE 1-8

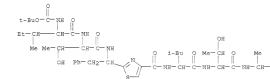


322 102409-CQ-7 CAPL/JS

CN 1-Allothreosinamide, N-[2-[1-[N-[N-(1,1-dimethylethoxy)carbonyl]-L-isoleucyl]-L-allothreosyl]amino]-2-phenylethyl]-4-thiazolyl[carbonyl]-L-leucyl-N-[2-[4-(methoxycarbonyl)-2-thiazolyl]ethyl]-, [R-[R*,R*]]- (9CI)
(CA INDEX NAME)

(ICA_INDEX_NAME)

PAGE 1-2



PAGE 1-7



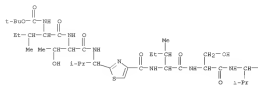
343 107070-70-0 CR0070

(2) L-serinamide.

N-[[[2-[1-[(N-{(1,1-dimethylethoxy)carbonyl}-L-isoleucyl)-

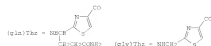
L31 ANSWER 50 OF 53 CAPLUS COPYRIGHT 2010 ACS on STM (Continued)
[1-[4-(methoxycarbonyl)-2-thiazolyl]-2-methylpropyl]-, [R-[R*,R*)]-
(9CI)
(CA INDEX NAME)

PAGE 2-2



PAGE 1-2

L31 ANSWER 51 OF 53 CAPLUS COPYRIGHT 2010 ACS ON STM
 ACCESSION NUMBER: 1986:627283 CAPLUS
 DOCUMENT NUMBER: 105237282
 ORIGINAL REFERENCE NO.: 105367274, 367304
 TITLE: Structural biochemistry. 23. Antineoplastic agents. 110. Synthesis of the dolastatin 3 isomer cyclo[1-Pro-L-Leu-L-Val-[R,D]-[gln]Thr-[gly]Thr]. Pettit, George R.; Holmsted, Gedric M. Cancer Res. Inst., Arizona State Univ., Tempe, AZ, 85287, USA.
 SOURCE: Journal of Organic Chemistry (1986), 51(24), 4580-5 CORREL. CORDY. ISSN: 0022-3263
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 OTHER SOURCE(S): CASREACT 105237283
 GI



AS The title cyclic peptide (I) was prepared by deblocking Boc-L-Leu-L-Val-[R,D]-[gln]Thr-[gly]Thr-L-Pro-OC(CH₂)₂Me, 4,5 (II, Boc = t-butyloxycarbonyl) by CF₃COOH and cyclizing the resulting Boc-deblocked peptide in THF containing pyridine. (I) was prepared by solution method. A comparison of synthetic I with natural dolastatin 3 showed that the natural peptide possesses a different amino acid configuration arising from some D epimers of the amino acid residues. IR and ¹H NMR data indicated that dolastatin 3 may contain D-Leu and D-[gln]Thr.

IT 104619-63-2P 104712-90-5P
 Re: ACT (Reactant); SM (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
 NH 104619-65-0 CAPLUS
 CH L-Valinamide, N-[[1,3-dimethylthio]carbonyl]-L-leucyl-N-[[4-amino-1-[4-[[[1,2-[[2,4,5-trichlorophenyl]amino]carbonyl]-1-pyrrolidinyl]carbonyl]-2-thiazolyl]methyl]amino]carbonyl]-2-thiazolyl]methyl]-, [S-(R*,S*)], mono(trifluoroacetate) (PCT) (CA INDEX NAME)

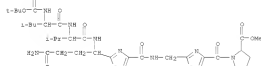
CH 1
 CHN 104619-64-3
 CMF C35 R43 C13 N6 OT 82

L31 ANSWER 51 OF 53 CAPLUS COPYRIGHT 2010 ACS ON STM (Continued)

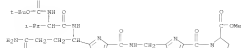
CH 2
 CHN 76-05-1
 CMF C2 R F3 G2



IT 92506-94-0P 104619-59-2P 104619-61-6P
 104619-62-7P 104619-63-8P 104712-82-5P
 104712-84-7P 104712-85-8P 104712-86-9P
 104712-87-0P 104712-88-1P 104712-89-5P
 XL 5PM (Synthetic preparation); PREP (Preparation)
 NH 92506-94-0 CAPLUS
 CH L-Valinamide, N-[[1,3-dimethylthio]carbonyl]-L-leucyl-N-[[4-amino-1-[4-[[[1,2-[[2-methoxy]carbonyl]-1-pyrrolidinyl]carbonyl]-2-thiazolyl]methyl]amino]carbonyl]-2-thiazolyl]-4-oxobutyl]-, [S-(R*,S*)], mono(trifluoroacetate) (PCT) (CA INDEX NAME)

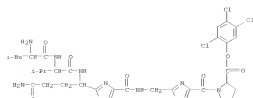


NH 104619-59-2 CAPLUS
 CH L-Proline, 2-[[2-[[[1,2-[[4-amino-3-[[[1,3-dimethylthio]carbonyl]amino]-2-methyl-1-oxoethyl]amino]-4-oxobutyl]-4-thiazolyl]carbonyl]amino]methyl]-4-thiazolyl]carbonyl]-, methyl ester, [S-(R*,S*)] (PCT) (CA INDEX NAME)



NH 104619-63-6 CAPLUS

L31 ANSWER 51 OF 53 CAPLUS COPYRIGHT 2010 ACS ON STM (Continued)

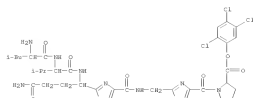


CH 2
 CHN 76-05-1
 CMF C2 R F3 G2



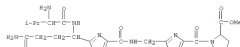
NH 104712-90-5 CAPLUS
 CH L-Valinamide, L-leucyl-N-[[4-amino-4-oxo-1-[4-[[[1,2-[[2,4,5-trichlorophenyl]amino]carbonyl]-1-pyrrolidinyl]carbonyl]-2-thiazolyl]methyl]amino]carbonyl]-2-thiazolyl]methyl]-, [S-(R*,S*)], mono(trifluoroacetate) (PCT) (CA INDEX NAME)

CH 1
 CHN 104712-89-2
 CMF C35 R43 C13 N6 OT 82



L31 ANSWER 51 OF 53 CAPLUS COPYRIGHT 2010 ACS ON STM (Continued)
 CH L-Proline, 2-[[2-[[[1,2-[[4-amino-3-[[[1,3-dimethylthio]carbonyl]amino]methyl]-4-thiazolyl]carbonyl]amino]methyl]-4-thiazolyl]carbonyl]-, methyl ester, [S-(R*,S*)], mono(trifluoroacetate) (PCT) (CA INDEX NAME)

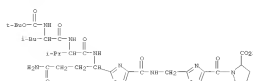
CH 1
 CHN 104619-60-5
 CMF C24 R33 N7 O6 82



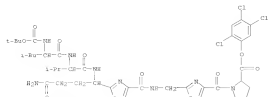
CH 2
 CHN 76-05-1
 CMF C2 R F3 G2



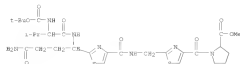
NH 104619-62-7 CAPLUS
 CH L-Valinamide, N-[[1,3-dimethylthio]carbonyl]-L-leucyl-N-[[4-amino-1-[4-[[[1,2-[[2-methoxy]carbonyl]-1-pyrrolidinyl]carbonyl]-2-thiazolyl]methyl]amino]carbonyl]-2-thiazolyl]-4-oxobutyl]-, [S-(R*,S*)], mono(trifluoroacetate) (PCT) (CA INDEX NAME)



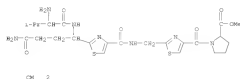
NH 104619-63-8 CAPLUS
 CH L-Valinamide, N-[[1,3-dimethylthio]carbonyl]-L-leucyl-N-[[4-amino-4-oxo-1-[4-[[[1,2-[[2,4,5-trichlorophenyl]amino]carbonyl]-1-pyrrolidinyl]carbonyl]-2-thiazolyl]methyl]amino]carbonyl]-2-thiazolyl]methyl]-, [S-(R*,S*)] (PCT)



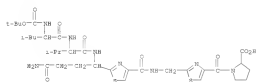
RE 104712-82-5 CAPLUS
CN L-Proline, 1-[[2-[[[2-[4-amino-3-[[2-[[[1,1-dimethyl-2-thiazolyl]carboxyl]amino]-2-methyl-1-oxobutyl]amino]-4-oxobutyl]-4-thiazolyl]carboxyl]amino]methyl]-4-thiazolyl]carboxyl]-, methyl ester, [S-(R*,R*)]- (9CI) (CA INDEX NAME)



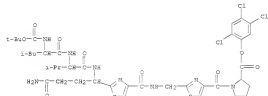
RE 104712-84-7 CAPLUS
CN L-Proline, 1-[[2-[[[2-[4-amino-3-[[2-amino-3-methyl-1-oxobutyl]amino]-4-oxobutyl]-4-thiazolyl]carboxyl]amino]methyl]-4-thiazolyl]carboxyl]-, methyl ester, [S-(R*,R*)]-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)
CN 1
CNS 104712-83-6
CNS C24 R33 N7 O6 S2



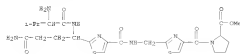
CN 2



RE 104712-88-1 CAPLUS
CN L-Valinamide, N-[[1,1-dimethylethoxy]carbonyl]-L-leucyl-N-[4-amino-4-oxo-1-[4-[[[4-[[2-[[2-(4,5-trichlorophenoxy)carbonyl]-1-pyrrolidinyl]carboxyl]-2-thiazolyl]methyl]amino]carboxyl]-2-thiazolyl]butyl]-, [S-(R*,R*)]- (9CI) (CA INDEX NAME)



RE 104757-49-5 CAPLUS
CN L-Proline, 1-[[2-[[[2-[4-amino-3-[[2-amino-3-methyl-1-oxobutyl]amino]-4-oxobutyl]-4-thiazolyl]carboxyl]amino]methyl]-4-thiazolyl]carboxyl]-, methyl ester, monohydrochloride, [S-(R*,R*)]- (9CI) (CA INDEX NAME)

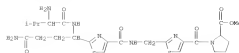


● SEE

CN 76-05-1
CNS C2 R F3 O2

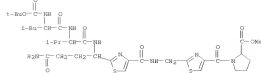


RE 104712-85-8 CAPLUS
CN L-Proline, 1-[[2-[[[2-[4-amino-3-[[2-amino-3-methyl-1-oxobutyl]amino]-4-oxobutyl]-4-thiazolyl]carboxyl]amino]methyl]-4-thiazolyl]carboxyl]-, methyl ester, monohydrochloride, [S-(R*,R*)]- (9CI) (CA INDEX NAME)



● SEE

RE 104712-86-9 CAPLUS
CN L-Valinamide, N-[[1,1-dimethylethoxy]carbonyl]-L-leucyl-N-[4-amino-1-[4-[[[4-[[2-(methoxycarbonyl)-1-pyrrolidinyl]carboxyl]-2-thiazolyl]methyl]amino]carboxyl]-2-thiazolyl]-4-oxobutyl]-, [S-(R*,R*)]- (9CI) (CA INDEX NAME)



RE 104712-87-0 CAPLUS
CN L-Valinamide, N-[[1,1-dimethylethoxy]carbonyl]-L-leucyl-N-[4-amino-1-[4-[[[4-[[2-(methoxycarbonyl)-1-pyrrolidinyl]carboxyl]-2-thiazolyl]methyl]amino]carboxyl]-2-thiazolyl]-4-oxobutyl]-, [S-(R*,R*)]- (9CI) (CA INDEX NAME)

(5 CITINGS)

L31 ANSWER 52 OF 53 CAPLUS COPYRIGHT 2010 ACS ON STM (Continued)
 ACCESSION NUMBER: 1986:579028 CAPLUS
 DOCUMENT NUMBER: 105:179229
 ORIGINAL REFERENCE NO.: 105:27904b, 27905a
 TITLE: Analog of dalaatatin 2. Synthesis, proton NMR studies, and spatial conformation
 AUTHOR(S): Barrier, Jean Luc; Roussin, Raymond; Benichart, Jean
 CORPORATE SOURCE: INSERM, Lille, 59045, Fr.
 SOURCE: Tetrahedron (1986), 42(19), 2695-702
 CUMUL: TETRAH; ISSN: 0040-4020
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 OTHER SOURCE(S): CASABACT 105:179209
 GI: For diagram(s), see printed CA issue.
 AB: Dalaatatin 3 analog 1 was prepared by deblocking
 Boc-Fro-Leu-Val-(gly)Thz-(gly)Thz-OMe (II; Boc = MeCOOC, NMe =
 neopentylidene) by HBr/ROAc and cyclizing the resulting
 Bz-Fro-Leu-Val-(gly)Thz-(gly)Thz-OMe, HBr in pyridine. Boc-Gly-NMe2
 underwent thiolation via the Lawesson procedure to give Boc-Gly(S)-NMe2,
 which was cyclized with CH3COCl to give Boc-(gly)Thz-OMe (III). III
 was Boc-deblocked by HBr/ROAc to give H-(gly)Thz-OMe.HBr (IV), whereas

L31 ANSWER 52 OF 53 CAPLUS COPYRIGHT 2010 ACS ON STM (Continued)

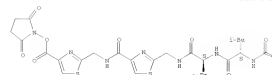
PAGE 1-3



IT 104728-43-2P
 RL: RCT (Reactant); SRN (Synthetic preparation); PREP (Preparation); RACT
 (Reactant or reagent)
 NH 104728-43-2 CAPLUS
 CN L-Valinamide, 1-[[[1,1-dimethylethoxy]carbonyl]-L-prolyl-L-leucyl-N-[[4-
 [[[(4-oxo-1-pyridin-2-ylmethylamino)carbonyl]-2-thiazolyl]methyl]-
 2-thiazolyl]methyl]amino]carbonyl]-2-thiazolyl]methyl]-
 2-thiazolyl]methyl]-1- (PCI) (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A

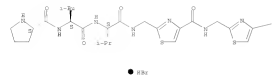


III was saponified to give Boc-(gly)Thz-OMe (V). V was coupled with IV by
 DCC/DMAP to give Boc-(gly)Thz-(gly)Thz-OMe, which was Boc-deblocked and
 then coupled with Boc-Fro-Leu-Val-OMe by DCC/DMAP to give
 Boc-Fro-Leu-Val-(gly)Thz-(gly)Thz-OMe, which was converted into II. A
 spatial mol. conformation of 1 was proposed based on 13 NMR spectroscopy.

IT 104728-46-3P
 RL: RCT (Reactant); SRN (Synthetic preparation); PREP (Preparation); RACT
 (Reactant or reagent)
 NH 104728-46-3 CAPLUS
 CN L-Valinamide, L-prolyl-L-leucyl-N-[[4-[[[4-[[[1,1-dimethylethoxy-3-
 pyridin-2-ylmethylamino]carbonyl]-2-thiazolyl]methyl]amino]carbonyl]-2-
 thiazolyl]methyl]-1- (PCI) (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A



● RBz



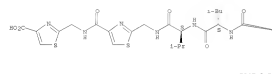
IT 104728-39-4P
 RL: SRN (Synthetic preparation); PREP (Preparation)
 (Preparation and esterification with hydroxypropanamide)
 NH 104728-39-4 CAPLUS
 CN L-Valinamide, 1-[[[1,1-dimethylethoxy]carbonyl]-L-prolyl-L-leucyl-N-[[4-
 [[[(4-oxo-1-pyridin-2-ylmethylamino)carbonyl]-2-thiazolyl]methyl]-
 2-thiazolyl]methyl]amino]carbonyl]-2-thiazolyl]methyl]-1- (PCI) (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-B

L31 ANSWER 52 OF 53 CAPLUS COPYRIGHT 2010 ACS ON STM (Continued)

Absolute stereochemistry.



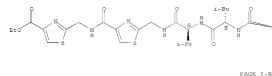
PAGE 1-B



IT 104728-39-3P
 RL: RCT (Reactant); SRN (Synthetic preparation); PREP (Preparation); RACT
 (Reactant or reagent)
 NH 104728-39-3 CAPLUS
 CN L-Valinamide, 1-[[[1,1-dimethylethoxy]carbonyl]-L-prolyl-L-leucyl-N-[[4-
 [[[(4-oxo-1-pyridin-2-ylmethylamino)carbonyl]-2-thiazolyl]methyl]-
 2-thiazolyl]methyl]amino]carbonyl]-2-thiazolyl]methyl]-1- (PCI) (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A



PAGE 1-B



IT 104728-40-7P

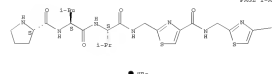
L31 ANSWER 52 OF 53 CAPLUS COPYRIGHT 2010 ACS ON STM (Continued)

RL: SRN (Synthetic preparation); PREP (Preparation)

NH 104728-40-7 CAPLUS
 CN L-Valinamide, L-prolyl-L-leucyl-N-[[4-[[[4-carboxy-2-
 thiazolyl]methyl]amino]carbonyl]-2-thiazolyl]methyl]-1- (PCI) (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A



● RBz

PAGE 1-B

—COOH

OS: CITING REF COUNT: 3 THERE ARE 3 CAPLUS RECORDS THAT CITE THIS
 RECORD (3 CITINGS)

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

AB Cyclic peptide 1 (R = COMED) (II), a proposed structure for delastatin 3, was prepared by deblocking peptide III (Roc = Me3COOC) by CF3CO2H, cyclization

the resulting Boc-deblocked peptide, and hydrolyzing the resulting 1 (R = OH). Thiazole IV was cyclized MeCOOOCMe to give thiazole V, which was cleaved by HCl to give thiazole VI (R = COMED, R2 = OH), which converted to VII (R1 = CH, R2 = Boc-[D]-Val-NE) (VII) in 5 steps. VII was Boc-deblocked and then coupled with

Boc-[D]-Pro-[D]-Leu-OH to give VI (R1 = CH, R2 = Boc-[D]-Pro-[D]-Leu-[D]-Val-NE), which was converted to III in 3 steps. II was not identical with delastatin 3. 91741:74-19

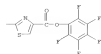
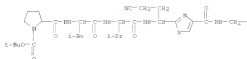
RE ECT (Isotant); SPM (Synthetic preparation); PREP (Preparation); RACT (Isotant or reagent)

[Preparation and deblocking-cyclization of]

91741:74-1 CAPLUS

CD D-Valanamide, 1-[[[1,1-dimethylethoxy]carbonyl]-D-prolyl-D-leucyl-N-[3-cyano-1-[4-[[[4-[[[4-(ethoxycarbonyl)-2-thiazolyl]methyl]amino]ethoxy]-2-thiazolyl]propyl]-, (R)- (9CI) (CA INDEX NAME)

PAGE 1-A



IT 91711:72-19

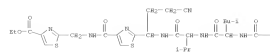
RE SPM (Synthetic preparation); PREP (Preparation)

[Preparation and saponification-pentafluorophenyl esterification of]

91711:92-1 CAPLUS

CD D-Valanamide, 1-[[[1,1-dimethylethoxy]carbonyl]-D-prolyl-D-leucyl-N-[3-cyano-1-[4-[[[4-[[[4-(ethoxycarbonyl)-2-thiazolyl]methyl]amino]ethoxy]-2-thiazolyl]propyl]-, (R)- (9CI) (CA INDEX NAME)

PAGE 1-A



PAGE 1-B



QS CITING REF COUNT: 2 THERE ARE 2 CAPLUS RECORDS THAT CITE THIS RECORD (2 CITINGS)

=> log y

COST IN U.S. DOLLARS

SINCE FILE

TOTAL

ENTRY

SESSION

FULL ESTIMATED COST

269.98

1694.79

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)

SINCE FILE

TOTAL

ENTRY

SESSION

CA SUBSCRIBER PRICE

-45.05

-53.55

STN INTERNATIONAL LOGOFF AT 15:17:38 ON 19 AUG 2010